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Field Measurement Program

GASCON2 Evaluation

October 1990



Field Measurement Program

GASCON2 Evaluation

FIELD MEASUREMENT PROGRAM

GASCON2 Evaluation

Volume 4

There are three other volumes:

FIELD MEASUREMENT PROGRAM - Volume 1
Atmospheric Dispersion Tracer Study Under Stable Conditions and Meteorological Study

FIELD MEASUREMENT PROGRAM - Volume 2
Appendices to Volume 1 - Appendix A

FIELD MEASUREMENT PROGRAM - Volume 3
Appendices to Volume 1 - Appendices B through D

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GASCON2 Model Evaluation Summary

Introduction

The Energy Resources Conservation Board (ERCB) commissioned Concord Environmental Corporation to develop the GASCON2 model in 1986. The model estimates the ground level H₂S and SO₂ concentrations and consequences in the event of an uncontrolled release from a well blowout or pipeline rupture. The ERCB also managed a Field Measurement Program where actual field data was collected in a simulated well blowout situation. This field data was then used to make comparisons to the following three models:

- | | |
|--|------------|
| • GASCON2 July 1990 Evaluation | Section 4 |
| • GASCON April 1990 Evaluation (on 1987 version) | Appendix A |
| • Simple Gaussian Evaluation | Appendix C |

All three model evaluations are contained in this volume, however this summary provides the results for GASCON2 in more detail with a comparison of GASCON2 to the simple Gaussian model. Generally, the GASCON2 model performed better than the original 1987 version of GASCON. The comparison to the simple Gaussian model showed that the performance depended on the source configuration and distance to receptor. It was for this reason that the GASCON2 evaluation was divided into an analysis of ground/elevated and by arc location.

The US Environmental Protection Agency (EPA) is one of the regulatory agencies with a published model evaluation protocol. The protocol was for evaluating time-averaged model predicted concentrations against field observations. However, the Field Measurement Program was designed to collect instantaneous data under passive dispersion conditions rather than time averaged data (see page E-7). Therefore, considerable effort had to be made to ensure that the most appropriate comparisons were made. Another important issue was the type of analysis. The EPA protocol was established for unpaired data analysis however, the field data collected appeared to lend itself to both a paired (in time and space) and unpaired data analysis. After the evaluations were complete, the highest level of confidence remained with the unpaired data analysis approach.

The most informative plots from all the evaluations are the Figures Sum.1 and Sum.2. These show the observed, simple Gaussian and GASCON2 normalized concentrations on one plot. The findings are discussed in that section.

Data Analysis and Reduction

The Field Measurement Program collected gas concentrations, plume spreads and meteorological data for both traverse (mobile) and stationary monitoring but only traverse data was used in this evaluation. A total of 846 traverses were made over 33 nights and corresponding model runs were made for each traverse. The predicted concentrations were compared to the 846 observed field concentrations. As mentioned, GASCON2 predicts three-minute concentrations and the tracer traverse data provides essentially instantaneous maximum concentrations.

Model performance can be measured using data sets where the predicted and observed values are either paired or unpaired in time and/or space. Paired analysis is useful if the data set is large and an understanding of the model's behavior is desired. This performance can be related to individual meteorological inputs. Comparisons involving values which are not paired in time and/or space are of particular use, when exact matching of meteorological inputs are not available or are uncertain and when the primary goal is to determine the ability of the model to predict the maximum concentrations that may occur. This evaluation addressed both of these methodologies however, as mentioned the unpaired proved to be most informative.

Model Evaluation Approach

GASCON2 (Alp *et al* 1990) is a computer-based model which can estimate exposure zones for an uncontrolled sour gas release under a number of different scenarios. Data obtained from the Field Measurement Program were used to evaluate this model's performance. In addition, comparisons were made to a simple Gaussian model which was used as a base model because of its simplistic nature.

Although GASCON2 is designed to address a number of different ignited (SO_2) and unignited (H_2S) scenarios, this evaluation only measures the performance of a vertical, steady state, H_2S release (mainly the passive dispersion module of GASCON2). The Field Measurement Program also collected stationary concentration fluctuation data which can be used to evaluate the consequence module of GASCON2 but the analysis of this data is not included in this evaluation.

Additionally, while tracer data was being collected, detailed on-site meteorological data were also collected over the entire test period. The meteorological pre-processing of this data was evaluated in Volume 1 and only general comments on its impact to GASCON2 are contained in this volume. GASCON2 has a module called METCAL that generates similar output to the pre-processor if it is given a value of surface heat flux.

The Field Measurement Program used sulphur hexafluoride (SF_6) as the non-toxic tracer gas. For model evaluation purposes, GASCON2 was altered to allow SF_6 to be the dispersant instead of H_2S or SO_2 . A main frame based model input processor was developed in order that batch runs of the model could be made quickly and efficiently.

GASCON2 Evaluation Results

The results of this evaluation were separated into the paired and unpaired analysis:

Paired Analysis

- The correlation between predicted and observed values was poor. The correlation coefficient (r) was 0.17 for ground release cases and 0.28 for elevated cases.
- When evaluating the percentage of predicted concentrations which fell within a factor of two of the observed, 23% of the ground cases and 40% of the elevated cases met this criteria.

- The paired data was sorted by concentration normalized by the release rate (C/Q). This analysis showed a trend towards increasing underprediction for the higher values of C/Q (worst case).

Unpaired Analysis

- The unpaired analysis showed much better results. The EPA model evaluation protocol, using a fractional bias method for the worst case regimes, was met for both ground and elevated releases at the 700 and 1 400 m arcs. (This protocol is based on the average of an arbitrary number of the highest predicted and observed concentrations being within a factor of 2).
- Plots of sorted normalized concentrations show that for worst case conditions (highest C/Q values), the model's predictions follow the trend of increasing observed concentrations. GASCON2 tends to track the observed C/Q values - See Figure Sum.1 and Sum.2.
- Unpaired analysis probably represents the most realistic evaluation of GASCON2 because of uncertainties in matching meteorological model inputs to the tracer data as well as meteorological classification of stability conditions.
- The GASCON2 dispersion module can predict worst case concentrations that might occur during a toxic release with reasonable accuracy (factor of 2).
- It is unclear if GASCON2 can predict plume concentrations at the correct place and time with the same level of accuracy.

Comparison

Figures Sum.1 and Sum.2 provide the best graphical representation from the entire set of model evaluations plots. These plots are based on the October 1990 version of the GASCON2 model. The model runs are based on 3-minute cross-wind dispersion (σ_y) values. The plots are normalized concentration (concentration divided by the flow rate = C/Q) versus the "percentage of cases".

Ground 700 m Arc

- The simple Gaussian tracked the observed until the higher level of C/Q values are reached. Then, they both track approximately in the same manor. It is believed that GASCON2 is not tracking well at the lower end because the model is forcing the neutral stability classification upon predictions that are known to be stable.
- Both models underpredicted slightly. Under prediction of concentration values has been considered serious in the past, given the concentration fluctuation and toxic load issues being dealt with in the consequence module of GASCON2. However, given the differences with respect to instantaneous versus time averaging, this may not be as large a concern.

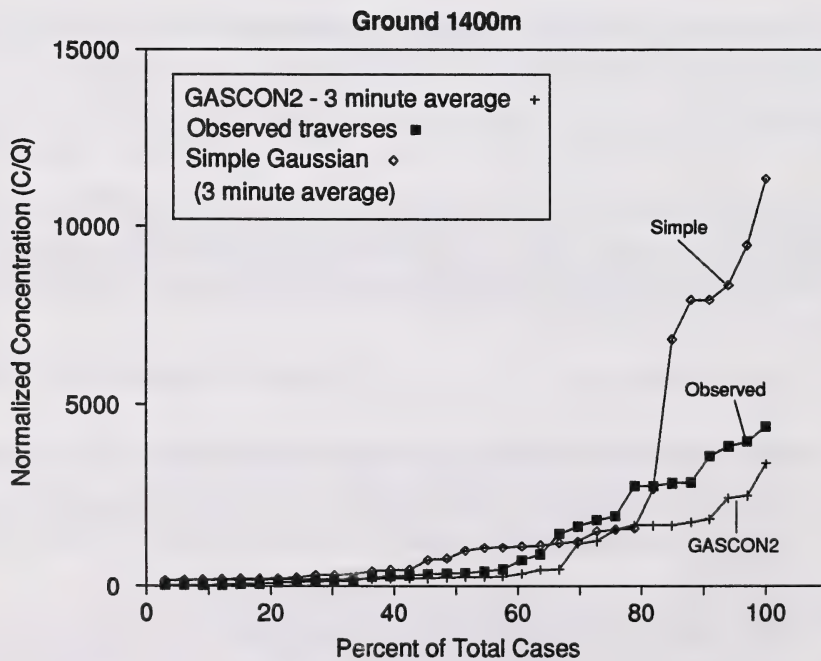
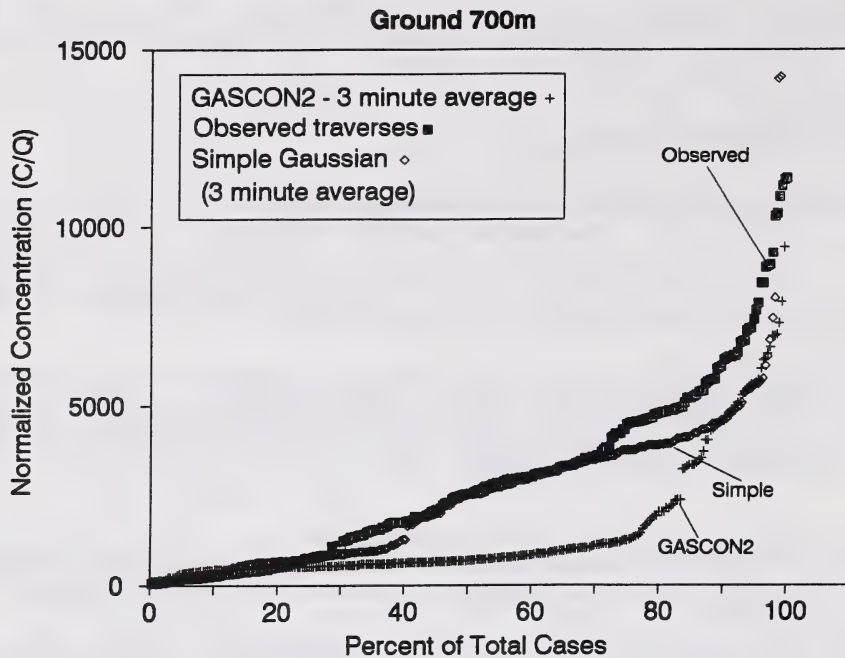


Figure Sum.1

Model Comparison For Ground 700 and 1 400 m Arcs.

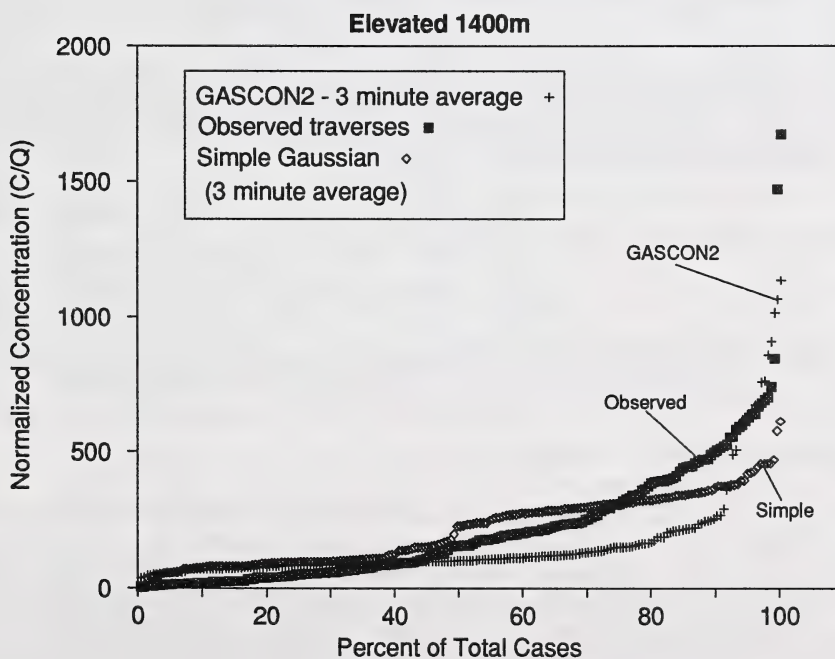
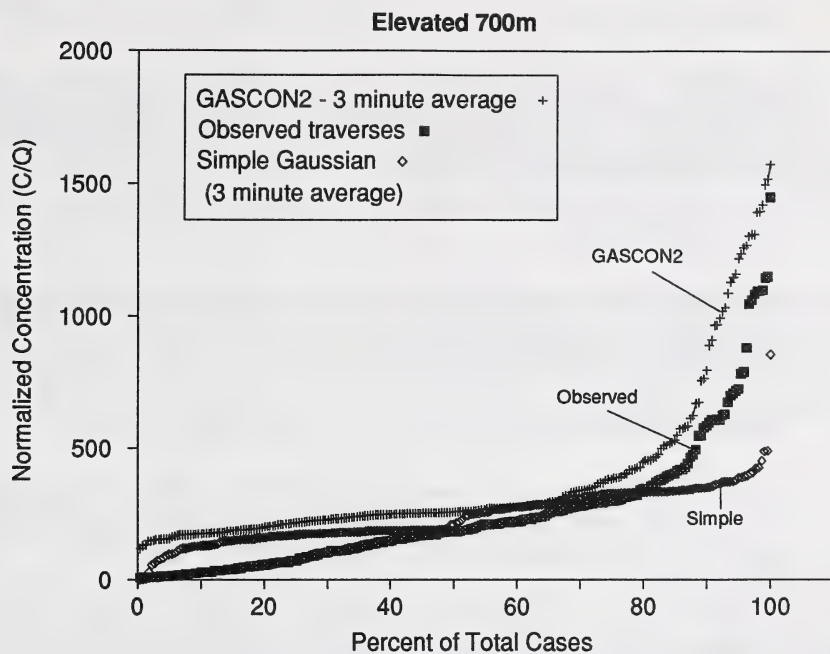


Figure Sum.2

Model Comparison For Elevated 700 and 1 400 m Arcs.

Ground 1400 m Arc

- GASCON tracked the observed values quite well but still slightly underpredicted. The simple Gaussian on the other hand overpredicted, significantly. Again, the same comment can be made on the underprediction issue with respect to time averaging.

Elevated 700 m Arc

- GASCON2 slightly overpredicted and tracked the observed very well for all concentrations. The simple Gaussian model crossed over the observed line and then underpredicted at high C/Q values.

Elevated 1400 m Arc

GASCON2 crossed over the observed line half way through the data set but overpredicted again at high C/Q values. The simple Gaussian model crossed over about the same point as GASCON2, but then underpredicted at the high C/Q values.

Generally, the "best performance" from a regulatory and public safety perspective would be to slightly overpredict in the high C/Q situation (worst case). In that regard, GASCON2 appears to out perform the simple Gaussian model especially for the elevated releases. In the ground case at 700 m, the simple Gaussian model was doing a better overall job of tracking the observed. This appears to be one of two possible problems with the GASCON2 modules, either the meteorological pre-processor or the ground based sigma y values. These are competing factors that could be looked at in more detail. An important factor to keep in mind is that historically there has been a much larger recorded incidence of the elevated releases compared to the ground case.

From other statistics in Section 4, you will note that GASCON2 was generally predicting within a factor of two (25 to 40% of the time). Modelling standards suggest that this is an excellent performance. It is interesting to note that the simple Gaussian model was also doing a reasonable job on the factor of two analysis. Since both models have Gaussian based assumptions, this provides some confidence in the simple approach. This should be good news to most atmospheric dispersion modelling scientists. The Gaussian based models are used by regulatory agencies throughout Canada and the United States. In any event, GASCON2 can handle other complexities such as jet expansion and concentration fluctuations, and this must be kept in mind.

This evaluation attempted to split the analysis into categories such as ground or elevated, however, further work could have been done on a case by case basis. Time permitted a review of the worst test night only (Test 15). The same general observations were made as for the entire data set. These were: underprediction until the high C/Q values are reached and then slight overprediction, but with reasonable tracking of the observed. This case study established even more confidence in GASCON2, especially for the highest concentrations. It was noted that the highest concentrations for Test 15 were at around 3 m/s rather than what was originally expected (<2 m/s). The summary of other test statistics are in Section 6 of Volume 1 and this same wind speed observation can be made for those tests even though some high concentrations were at lower wind speeds.

Averaging Time Considerations

Difficulties exist with trying to run a model as it would normally be run with 3-minute averaging time sigmas, and then comparing predictions to instantaneous observations. To emphasize that point, the ground release at the 700 m arc was plotted for various averaging times. Since the exact time cannot be assigned to the observed instantaneous concentrations, the observed line on the plot is identified as "assumed instantaneous". Practically speaking, the time would be around 1 to 30 seconds.

Both the simple Gaussian and the GASCON2 models were run at different sigma averaging times (one hour, 3-minute and 30-seconds); in an effort to approach instantaneous predictions. The graphs are not directly comparable however, if the shorter averaging times are used, the plot shows that model predictions would be closer to the observed. This could alleviate any concerns regarding underprediction for the ground, 700 m case. Unfortunately, this would also have a similar effect on the elevated case.

Comments

GASCON2 development has taken four years to reach completion. All of the modules have undergone scientific investigation and sensitivity testing by both the ERCB and Concord staff. The program was also under the scrutiny of the Field Measurement Program Technical Committee and Scientific Advisory Board. Additionally, the passive dispersion and meteorological pre-processing modules have had the added benefit of being evaluated against actual field measurements.

Given the situation, this October 1990 version of GASCON2, was the best effort, to incorporate the complex scenarios that the model was designed for. Therefore, the recommendations for further model enhancement, outlined here, are to be thought of as future considerations when research in these areas moves the science forward. This could take some time and meanwhile it is believed that this model evaluation has shown there is sufficient confidence to use the model as it now stands.

Suggested Review/Enhancements

- Review the stability classification criteria. The model appears to be forcing a neutral classification when a stable classification was observed.
- Investigate the GASCON2 sigma y formulations as the predicted sigma y appears to be more constant than the observed values. This could be tied to the neutral stability classification issue as neutral formulations are more constant.
- Investigate the ground based dispersion formulation. GASCON2 assumes Gaussian in the cross-wind direction, but not in the vertical direction. Since the simple Gaussian model tracked the observed better than GASCON2 for the ground 700 m arc, it may be worth changing the GASCON2 formulation. Since this and the above factors may have competing effects, this change may not be necessary.

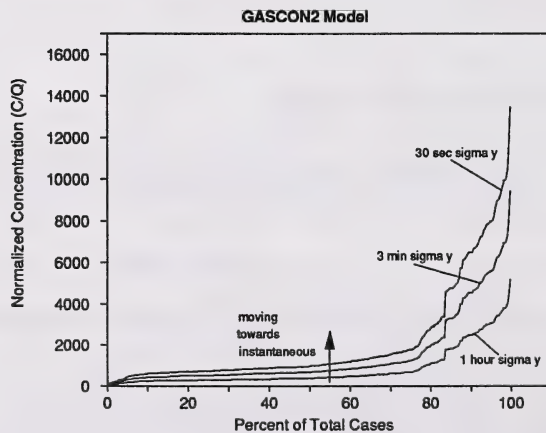
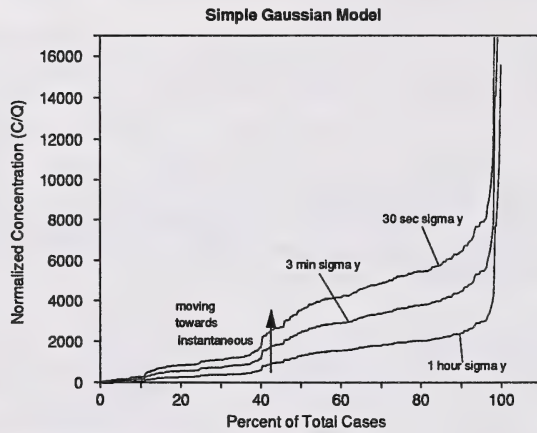
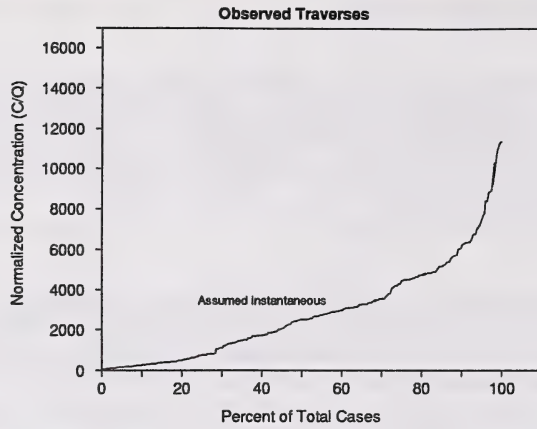


Figure Sum.3

The Importance of Averaging Times (Ground at 700 m).

Conclusions

The comments identify areas for improvement and not surprisingly the Field Measurement Program findings came to similar conclusions. Note that the enhancement suggestions are all for the ground based releases near the source and should be looked at together. The suggestions from both Volumes 1 and 4, warrant some further attention; however, the confidence in GASCON2 was substantially increased with the field work and the model can be used in its current form.

GASCON2 performed reasonably well for all the cases considered. The performance was particularly good for the most important cases, those under consideration for public safety. Generally, it out performed the simple Gaussian model and tended to track the field observations better. The fact that GASCON2 has many other modules and can deal with a wide range of release scenarios must also be kept in mind. This evaluation was for the passive dispersion module only.

Keep in mind that the ground based release is the most infrequent historical event and that most releases are expected to be elevated. This observation should be put into perspective before any effort is made to enhance the model. All future model changes, after the public release in October, will be reflected in the GASCON2 User's Guide, Volume 8, as updates are generated. Further details of all evaluations are contained in this volume.

1 INTRODUCTION

1.1 Background

The Energy Resources Conservation Board (ERCB) is responsible for approving applications for new energy projects and for regulating the operation of existing energy facilities in the Province of Alberta. In assuming this role, the ERCB is also responsible for providing advice and information on Alberta energy related-issues to industry, government and the public.

Natural gas is an extremely important energy resource for the province of Alberta. Somewhat more than half of this natural gas is derived from sour gas reserves which contain hydrogen sulphide (H_2S). The H_2S content of commercial sour gas reserves in the province of Alberta can vary from a few parts per million (ppm) to more than 50 per cent. As a consequence, sour gas has to be treated with respect since high concentrations of H_2S are extremely toxic (~ 600 to 1 000 ppm by volume) and low concentrations (20 to 50 ppm by volume) can be irritating to the lungs, nose, throat and eyes (Barr 1988).

For this reason, the ERCB has strongly enforced policies regarding sour gas emergency planning zones and the establishment of appropriate setback distances for sour gas facilities which include wells, pipelines and processing plants. Safeguard guidelines have been established using a combination of predicted atmospheric dispersion behaviour, risk assessment methods, judgement based on sour gas releases from blowouts and pipeline ruptures, and the results of field simulations of sour gas releases (APIGEC 1974, 1978, 1979 and Atwell 1979). The provincial subdivision approving authorities have adopted the same setback distances as the ERCB through the Subdivision Regulations pursuant to the Planning Act (ERCB ID 79-2, ID 81-3, ID 87-2, IL 88-9 and IL 88-9 Amendment, ERCB Enerfax 6 and 7, Alberta Municipal Affairs 1986, Alberta Public Safety Services 1985, Canadian Petroleum Association 1987).

Drilling for, producing, transporting and treating sour gas has always presented a number of difficulties including: fouling and coagulation of drilling fluids, rapid stress corrosion cracking of metals and, if released into the atmosphere, extreme toxicity to humans and animals through inhalation. Over the years, improved design of drilling equipment and procedures, improved H_2S resistant pipelines, improved process plant metallurgy, special emergency alarms and shut-down and control procedures have been implemented. These improvements in the handling of sour gas have qualitatively reduced the risks to industry workers and members of the public by reducing the incidences and occurrences of sour gas releases.

Despite these achievements, public concern regarding sour gas has grown, particularly because of the 1982 Lodgepole sour well blowout and increased sour gas developments near populated areas (Sage 1985). The Lodgepole blowout vented $2800 \times 10^3 \text{ m}^3/\text{d}$ of sour gas containing 25% H_2S and was out of control for 60 days. H_2S concentrations of 10 ppm were recorded on monitors 22 kilometres (km) from the well. H_2S odours were observed in the cities of Edmonton (140 km) and Calgary (240 km) (ERCB D 84-9).

Public concerns over the Lodgepole blowout and other proposed sour gas development in populated areas prompted the ERCB to commission Concord Scientific Corporation (now Concord Environmental Corporation), in 1986, to develop a dispersion model and risk approach specific to sour gas releases. Originally this was to result in two models, GASCON

and GASRISK. Model development methodology and results were subject to scientific peer review and public scrutiny. The scientific peer review group was called the Scientific Advisory Board. A communications plan was established to ensure the study and the views of the Scientific Advisory Board would become public knowledge (ERCB Newsletters 1986 to 1987). The draft GASCON model results were presented to the public in June 1987 (Alp *et al* 1987). Meanwhile the risk work carried on, developing an approach to incorporate the results of GASCON.

The GASCON computer model was specifically designed to simulate the initial behaviour and dispersion of sour gas plumes. The model addressed releases from either a well blowout or a pipeline rupture and from either an ignited or unignited plume. The GASCON model handled a range of source configurations, such as horizontal or vertical jets. For typical Alberta conditions, the GASCON model predicted large H₂S concentrations under low turbulence conditions.

Scientists reviewing the Concord Scientific 1987 results held differing views on the predicted H₂S concentrations. Some thought the GASCON model predictions would have been smaller, thus posing less public risk if dispersion based on site-specific turbulence observations were used; others thought that the concentrations would be larger if very quiescent "worst case" atmospheric conditions could be simulated by the model.

To resolve this conflict of opinion, a proposal was submitted to the ERCB recommending that risk work be delayed until a field measurement program could be completed to more fully evaluate and verify the GASCON model. The ERCB took this proposal to all the involved parties, including the public, government and industry, and found that all were in favour of the field program. The ERCB, in response to the favourable comments, initiated a field measurement program to evaluate low wind speed, stable atmospheric conditions. The public was advised of the program (ERCB Newsletters 1988) and informed that the final GASCON model and risk work would be complete after the results of the Field Measurement Program could be incorporated.

The Field Measurement Program started in 1988 and was completed by 1990. Details of the Field Measurement Program are contained in this Volume 1 along with an analysis of the results. The appendices for Volume 1 are presented as Volumes 2 and 3. A review of the field analysis results indicated that certain GASCON assumptions should be changed. These changes were incorporated into a GASCON2 model so that an evaluation of the passive dispersion portion of GASCON2 could be undertaken using the field data. Those model evaluation results are in Volume 4.

Additionally, the GASCON and GASRISK models were integrated into the single GASCON2 model. The enhanced GASCON2 model can now predict concentrations and consequences and is referred to as GASCON2 (Alp *et al* 1990 - Volume 5). The risk approach that was being developed by Concord Environmental Corporation over the same time period incorporates the results of GASCON2 and is documented in Alp *et al* 1990 - Volume 6 and ERCB - Volume 7.

The first seven volumes that have been mentioned in this section refer to the Field Measurement Program, GASCON2 and the risk approach. There are three other related documents. Volume 8 is the GASCON2 User Guide. Volume 9 is the Scientific Advisory Board Commentary on Volumes 4, 5 and 6. Volume 10 is a Summary of the ERCB and Concord Environmental Volumes. Since all documents, including those of the ERCB, Concord and the Scientific Advisory Board, were to be made public, the ERCB packaged the ten volume set and released all volumes in October 1990.

1.2 Field Measurement Program Administration

1.2.1 Organization

The Field Measurement Program organization chart is shown in Figure 1.1. Primary responsibility for the management of the program was assumed by the ERCB with co-operation from industry and government.

A Program Management Committee was established in late 1987 to oversee the general co-ordination, administration and direction of the project. The Management Committee was comprised of three members: an ERCB representative (chairman), a public representative from the City of Calgary and an industry representative from the Canadian Petroleum Association.

A Technical Committee was also appointed by the ERCB in late 1987 to determine the technical scope and conceptual design for the program data collection, reduction and analysis portion. The eight-member Technical Committee was comprised of representatives from the ERCB (chairman), University of Alberta, Alberta Environment, the community and industry members representing the Canadian Petroleum Association, the Independent Petroleum Association of Canada and the Small Explorers and Producers Association of Canada. The selected conceptual Field Measurement Program design was submitted to and approved by the Management Committee. The Technical Committee was not involved in the design of the model evaluation.

In June 1988, tender invitations from consulting organizations located in Western Canada and the United States were requested to carry out the field program. In August 1988, a contract was awarded to Concord Scientific Corporation (now Concord Environmental Corporation) with Promet Environmental Group and Indaco Air Quality Services acting as sub-contractors.

The Field Measurement Program co-ordinator was Lynda Holizki (ERCB) who was assisted by:

- Vic Bohme, who acted as field program manager,
- Mervyn Davies (Concord), and Touche Howard (Indaco) who acted as primary technical consultants,
- George Kupfer and Jack Bales (ERCB), who acted as communication co-ordinators, and
- The Technical Committee and many ERCB staff.

All individuals have been identified in the acknowledgment section.

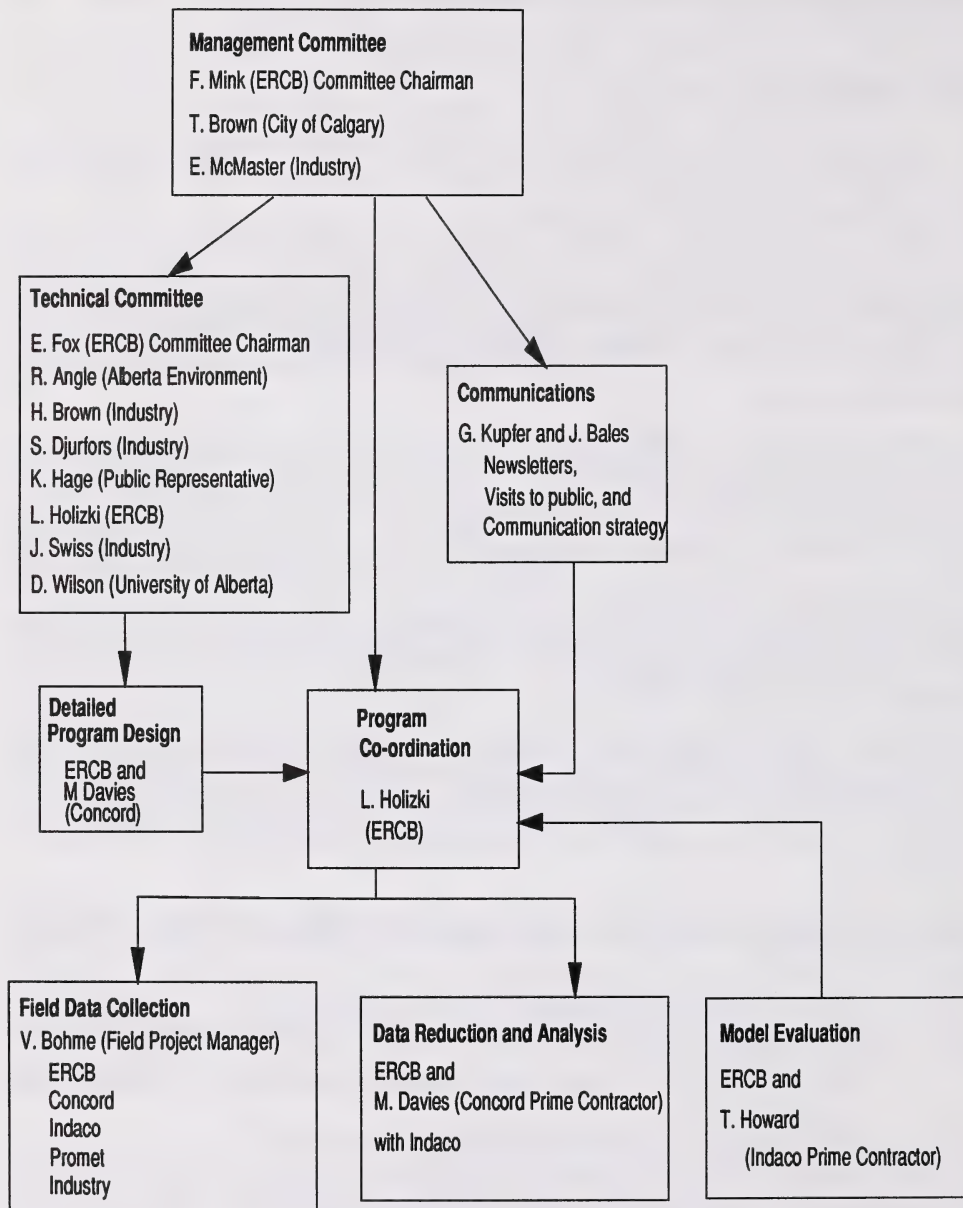


Figure 1.1
ERCB Field Measurement Program Organization Chart.

1.2.2 Program Contributions

To assist with the execution of the Field Measurement Program, the data reduction and data analysis, resources from within the ERCB, Alberta Environment, industry and local public were available. Table 1.1 summarizes the contributions from these sectors. The significant industry contribution provided the essential support. Without it, the project would not have had the initial backing to see it to completion. It is worth noting that the industry contribution came forward on the premise that the field data would be generic in nature, meaning that the data could be used for any model evaluation.

Additionally, work contracts to assist with the field data collection were offered to local residents. For example, local residents acted as drivers for the analyser trucks and a local person painted field and survey signs. It is worth noting that the contributions came forward so that field results would be generic to ensure that a model evaluation could be done.

1.3 Program Data Reduction and Analysis Approach

The Technical Committee reviewed the GASCON report and confirmed that, indeed, the low turbulence atmospheric condition warranted the most attention when predicting the behaviour of an accidental release of H₂S. More specifically, the Technical Committee agreed that most previous research efforts focused upon modelling and monitoring mean concentrations (usually 1-hour averages) downwind of a toxic source for neutral or unstable conditions.

Unfortunately, a mean concentration averaged over minutes or hours is not adequate to estimate the potential damage to a human who may be sensitive to instantaneous, high concentrations. In particular, downwind of a narrow meandering plume, a receptor receives intermittent doses of the pollutant (separated by periods of uncontaminated air) as the plume sweeps back and forth amid large-scale wind direction changes. If the scales of the meandering motions are much larger than the scale of the instantaneous plume, the plume does not impact the receptor very often, and a mean concentration at the receptor is low. On the other hand, the concentrations within the instantaneous plume may be high enough to kill an exposed person. Therefore, plume meander and concentration fluctuation are critically important. The Technical Committee agreed that predicting the short term peak concentrations under low turbulence conditions was essential and summarized the issue as follows:

- To improve the understanding of meandering plumes, experimental data are required since the process which describes the transport and dispersion of plumes is not clearly understood theoretically. Of the public data in existence, most have been collected in wind tunnel studies where plumes do not meander, and none of the data collected in full-scale studies contain simultaneous concentration and wind measurements.

To address this issue, the Technical Committee and project team designed and implemented a generic field program consisting of two parts:

Table 1.1
Organizations Contributing to the Project

Organization	Contribution
Energy Resources Conservation Board	Management, manpower and office services
Canadian Petroleum Association (CPA), Independent Petroleum Association of Canada (IPAC) and Small Explorers and Producers Association of Canada (SEPAC)	\$500 000
TransAlta Utilities Corporation	\$10 000
Alberta Power	\$5000
Shell Canada Resources Limited	Office trailers, 4x4 truck, colour photo-copying and radios
Alberta Environment	Equipment and manpower
Canadian Petroleum Association (CPA)	Radios, tents, generators and mechanic
Synchrude Canada Ltd.	Tethersonde and an AC power conditioner
Alberta Public Works, Supply and Services	Vehicle rental
Petro Canada Inc.	Fuel (\$5100)
City of Calgary, Parks and Recreation	Snow-blower fan
Gulf Canada Resources	Video Editing Assistance
Mount Royal College, Department of Chemical and Biological Services	Acoustic sounder
Esso Resources Canada Limited	Surveying (1 week)
Canadian Occidental Petroleum Ltd.	Computers, manpower and meteorological data
Amoco Canada Petroleum Company Ltd.	Meteorological data
Kananaskis Center for Environmental Research, University of Calgary	Meteorological data
Environment Canada, Atmospheric Environment Service	Meteorological data
University of Calgary, Department of Geography	Meteorological data

- **Tracer Study**

During an intensive study period, a sulphur hexafluoride (SF₆) tracer gas was released into the atmosphere. This tracer gas released during low wind speed conditions when downstream concentrations reach a maximum. Actual downstream concentrations were monitored and data recorded at several downstream distances. Concentration data collected were used to establish the behaviours and patterns associated with plume dispersion. Meteorological data, concurrent with each tracer release, were obtained to aid in the interpretation of the tracer gas results; and

- **Meteorological Study**

Atmospheric turbulence and profile data were collected and used to obtain meteorological information on the frequency and persistence of low turbulence atmospheric conditions.

The Field Measurement Program was conducted over reasonably flat terrain approximately 20 km from the city of Calgary. The tracer release and sampling occurred during the months of October, November and December 1988. Tracer tests were performed whenever low wind speed/stable conditions were expected. The diffusion meteorological station commenced operation in October 1988 and continued to operate until a full 12-month set of meteorological data as collected. The data analysis component of the study was completed in mid 1990. An overview of the program can be found on the following pages.

1.4 Program Data Reduction and Analysis Objectives

1.4.1 Tracer Objectives

The tracer section of the Field Measurement Program involves extraction and analysis of plume concentration data. Data were collected while monitoring under two conditions; traverse (continuous mobile monitoring while travelling through the plume) and stationary (continuous monitoring while stationary in the plume).

Objectives for the tracer component of the study include:

- An assessment of the frequently used Gaussian plume approximation for describing the cross-wind concentration profile in the plume.
- The identification of the conditions which resulted in the smallest cross-wind spreads.
- An evaluation of the instantaneous and time-averaged cross-wind spreads compared with predicted values.
- A determination of peak-to-mean concentration ratios for the stationary concentration data.
- A comparison of predicted and observed plume centreline concentrations using a simple Gaussian plume model.

The analysis of the data focused on all the data collected with a limited review of case studies.

1.4.2 Meteorological Objectives

The meteorological station collected data for a full 12 month period (October 1988 to October 1989). Meteorological objectives identified for the Field Measurement Program include:

- The preparation of a climatological summary of important selected and derived meteorological parameters for the Field Measurement site.
- The evaluation of turbulence-related variables in the atmospheric boundary layer which are responsible for dispersion processes.
- An evaluation of the occurrence and persistence of low wind speed conditions.
- An evaluation of various meteorological preprocessor schemes ranging from those based on the STAR analysis of airport observations to those based on the determination of boundary layer parameters.
- The determination of the spatial representativeness of meteorological observations at various locations in the vicinity of the study area.
- An evaluation of the empirical power laws used to convert turbulence levels from one averaging period to another.
- A comparison of wind and turbulence data collected from sonic anemometers with those collected from conventional propeller anemometers.
- The determination of on-site mixing heights.

For the purposes of analysis, the data were grouped into two 6-month blocks: winter (October 1988 to March 1989) and summer (April 1989 to October 1989). For most of the objectives, the full 12-month data were used while for some, only the winter data were used.

1.5 Model Evaluation Approach

The Field Measurement Program generated gas concentrations, plume spreads, and meteorological data which could be utilized for model performance comparisons. These comparisons focussed on GASCON2 (Alp *et al*, 1990), a model developed by Concord Scientific Corporation. However, comparisons were also made to a generic Gaussian dispersion formulation which was used as a control model because of its simplistic nature. The evaluations are the subject of this Volume 4 with the focus being on GASCON2.

1.5.1 Simple Gaussian Model Evaluation Approach

Details of the simple Gaussian relationship are contained in Appendix C, along with a model comparison. Five different sets of field plume spread data were used in the Gaussian model comparison and the fifth option was further broken into ground and elevated releases.

1.5.2 GASCON2 Model Evaluation Approach

GASCON2 is a computer-based model which can be used to estimate exposure zones and lethality consequences for uncontrolled sour gas releases, under a number of different scenarios. The model can address both steady state and transient release cases for both H₂S

1.5.2 GASCON2 Model Evaluation Approach

GASCON2 is a computer-based model which can be used to estimate exposure zones and lethality consequences for uncontrolled sour gas releases, under a number of different scenarios. The model can address both steady state and transient release cases for both H₂S (unignited) and SO₂ (ignited) situations as well as horizontal and vertical releases. GASCON2 has the capability to handle more complex situations but the Field Measurement Program was only designed to test passive dispersion. For this model performance evaluation only the modules of the model that deal with steady unignited vertical releases were utilized and compared to the field traverse data.

It should also be noted that the GASCON2 consequence module is not directly evaluated with the Field Measurement Program data. The concentration fluctuation subroutine is contained in the consequence module and although stationary data was collected for further understanding of concentration fluctuations, the analysis of this data was not included in this evaluation.

Sulphur hexafluoride was the nontoxic tracer gas released in the Field Measurement Program. Therefore, the GASCON2 input was altered to use sulphur hexafluoride (SF₆) as the dispersant instead of H₂S or SO₂ for model evaluation purposes. A model input preprocessor was developed to allow GASCON2 to be run in batch mode utilizing varying field input parameters. Field meteorological parameters such as surface friction velocity, Monin-Obukhov length, temperature gradient, σ_v and σ_w , all could be incorporated as inputs into GASCON2. GASCON2 was only evaluated using minimum field inputs. However, the 1987 version of GASCON was tested with a varying number of inputs (see Appendix A).

The GASCON2 modifications and procedures for use with SF₆ are discussed in Section 3. The GASCON2 model evaluation is contained in Section 4.

1.6 Model Evaluation Objectives

1.6.1 Simple Gaussian Model Evaluation Objectives

The simple evaluation was done to serve as a base case evaluation which will also aid in understanding what impact the various plume dispersion coefficients have on GASCON2 predictions.

- Field Measurement Program concentrations were compared to the simple model using various plume dispersion rates. The options for plume dispersion coefficients include those used by Alberta Environments (σ_y and σ_z), horizontal dispersion coefficients determined from FMP tracer traverse data (σ_y), and dispersion coefficients derived from turbulence parameters measured by the FMP meteorological tower (σ_v and σ_w).

All results appear in either tabular or graphical format in Appendix C.

1.6.2 GASCON2 Model Evaluation Objectives

The objective was to evaluate the passive dispersion module of the GASCON2 model, primarily under low wind speed stable conditions. This objective was undertaken in a number of defined steps:

For Paired Data

- The comparison of Field Measurement Program concentrations to the 1987 GASCON predicted concentrations under three possible input options:

- Option 1 With GASCON generated surface friction velocity (U^*), Monin-Obukhov length (L) and Temperature Gradient.
- Option 2 Field U^* , L and Temperature Gradient.
- Option 3 Field σ_v and σ_w .

All results appear in Appendix A.

For Paired and Unpaired Data

- The evaluation of the August 1990 version of GASCON2 using typical comparisons of predicted and observed concentrations. These comparisons were made with data sets that were both paired and unpaired in time and space.
- The evaluation of ground and elevated formulations to determine any release based deficiencies.
- To examine unpaired normalized concentrations to determine the ability of the model to predict the highest range of concentrations that may result from a release.
- To apply the Environmental Protection Agency (EPA) established model evaluation protocol to GASCON2.
- To evaluate the ability of the model to calculate plume dispersion coefficients.

All results appear in either tabular or graphical format in Section 4, Volume 4.

1.7 Field Measurement Program Schedule

The project schedule can be subdivided into pre-field activities, field activities and data reduction activities:

Pre-field Activities

Management Committee appointment	November 1987
Technical Committee appointment	December 1987
Tender invitation	June 1988
Contract award	July 1988

Field Activities

Installation of hardware	August to September 1988
Field tests	October to December 1988
Tracer hardware decommissioning	January 1989
Meteorological hardware decommissioning	October 1989

Data Reduction Activities

Data reduction (tracer)	February to September 1989
Data reduction (meteorology: winter)	February 1989 to March 1990
Data analysis (tracer and meteorology)	September 1989 to March 1990
Data reduction (meteorology: summer)	February to June 1990
Data analysis (meteorology: summer)	June to August 1990
Simple Gaussian model evaluation	January to April 1990
1987 GASCON evaluation/enhancement	January to August 1990
GASCON/GASRISK integration	April to August 1990
GASCON2 model evaluation	August to September 1990

The extended schedule presented project management challenges to ensure continuity and minimize prolonged resource conflicts.

1.8 Field Measurement Program Reports

There are four reports associated with the Field Measurement Program:

Field Measurement Program

Atmospheric Dispersion Tracer Study Under Stable Conditions and Meteorological Study.

Volume 1

Field Measurement Program

Atmospheric Dispersion Tracer Study Under Stable Conditions and Meteorological Study.

Volume 2 - Appendices to Volume 1

Field Measurement Program

Atmospheric Dispersion Tracer Study Under Stable Conditions and Meteorological Study.

Volume 3 - Appendices to Volume 1

Field Measurement Program

GASCON2 Evaluation.

Volume 4

Volume 1 discusses the design and provides a description of the Field Measurement Program data collection procedures. This is followed by the presentation of the results for the tracer and meteorological components of the program. Volumes 2 and 3 are appendices to Volume 1 and include detailed plots and data for the tracer component of the study. The appendices also provide additional background data on the details of certain aspects of the program. This Volume 4 provides an assessment of a simple Gaussian model and the GASCON2 model based on the Field Measurement Program observations. It also includes an appendix on the 1987 GASCON evaluation.

2 GASCON EVALUATION AND CHANGES

2.1 Introduction

There were two earlier public releases of GASCON. The first in June 1987 and the second in April of 1990. The only model evaluation possible in 1987 was a preliminary assessment of how well GASCON predicted the Lodgepole concentrations. By 1990 the Field Measurement Program was complete and more rigorous evaluations were done. The Field Measurement Program was designed to gather data for the steady state passive dispersion region, therefore only one module of GASCON could be evaluated.

The April 1990 evaluation was on the 1987 version of GASCON. This evaluation was for the purpose of comparing GASCON to the field data prior to making any adjustments to the model. At that point none of the Field Measurement Program findings were incorporated. During that intensive review and running of the model both Concord and ERCB staff adjusted modules to more accurately reflect the physics of the situation. The model also started to incorporate other modules such as the consequence model and with all of the changes the model was given a new name, GASCON2. By July of 1990 it was thought that all changes that were going to be required were made. The GASCON2 model was then re-evaluated and that evaluation is the subject of Section 4.

Since July 1990 there were two other minor model adjustments. These were with the ground based plume spreads and the jet expansion drag factor. A number of sensitivity runs were made to assess the potential impact of these factors on the July 1990 evaluation. It was found that the impact was minimal and therefore no further evaluation was warranted. The July 1990 evaluation was then deemed to be a fair assessment of the final October 1990 GASCON2 model. Details of the 1987 to 1990 changes are outlined in Section 2.2.

As mentioned, the Field Measurement Program was designed for steady state passive dispersion only. One of the best ways to test the passive dispersion module of a complex model like GASCON2 is to check it against a simple Gaussian model. GASCON2 itself assumes Gaussian formulations for all but the ground releases where it assumes a Gaussian distribution in the cross-wind and an exponential distribution in the vertical direction. The GASCON2 assumptions are different from the simple model and these are identified in Section 4. A comparison of a simple Gaussian model to GASCON2 was made and the results appear in the summary at the start of this volume. The fact that GASCON2 can handle other complex physical situations with its other modules must be kept in mind when reviewing the comparisons in the summary.

The simple Gaussian evaluation and the earlier GASCON (1987 version) model framework and evaluation appear in the appendices of this volume for quick reference.

Appendix A	GASCON (1987 Version) Evaluation
Appendix B	GASCON (1987 Version) Model Framework
Appendix C	Simple Gaussian Evaluation

These early evaluations helped focus on the important issues to deal with in the GASCON2 model evaluation. They were primarily done on a paired data analysis basis rather than an unpaired basis. The paired analysis proved to be the least informative of the two options, therefore the GASCON2 evaluation was focused on the unpaired data analysis. Generally GASCON2 performed better than GASCON after all changes had been made. As far as the comparison to the simple Gaussian model performance depends on the type of release.

2.2 GASCON Becomes GASCON2

This section only provides a brief summary of the model changes. The detailed explanation of equations and variables can be found in Volume 5, GASCON2 - A Model to Estimate the Ground-level H₂S and SO₂ Concentrations and Consequences from Uncontrolled Sour Gas Releases. The following summary provides a quick overview of those changes.

GASCON Changes Since June 1987 Version (For July 1990 GASCON2 Evaluation)

Impact on July Evaluation

Findings from the Field Measurement Program

- | | |
|---|-------------------------------|
| • Changing the power law exponent used to convert meteorological turbulence measurements from one averaging time to another, to 0.20. | Code change. |
| • Confidence in the Briggs formulations obtained through smoke tests. | Code change. |
| • Acknowledging that the GASCON formulations incorporate U^* , Z and L and these were providing for minimum turbulence. | Helpful but no code change. |
| • Understanding the frequency, persistence and duration of low wind speeds. | Incorporate in risk approach. |

Findings from the Field Measurement Program that warrant further investigation and have not been incorporated.

- | | |
|--|-----------------------------|
| • Information on the wind shear enhancement correction factors. | Helpful but no code change. |
| • Understanding the limitations of the meteorological preprocessing (it tends to identify more neutral stability classes than found in the field). | Helpful but no code change. |
| • Information on the minimum stable values for U^* , Z and L . | Helpful but no code change. |

Changes due to model review and running.

- | | |
|---|-------------------------------|
| • Adoption of the Triple-Shifted Rijnmond Parameters. | Incorporate in risk approach. |
| • Changed the plume penetration assumptions in stable atmospheres to unlimited mixing. | Code change. |
| • Adjusted plume rise stopping criteria for velocity and dense gases. Model can run dense gases and gives lower plume rise for stable conditions. | Code change. |
| • Addition of reflection terms from inversion lid in neutral and unstable atmospheres. | Code change. |
| • Slight changes in the averaging time used for plume spreads in stable atmospheres. The original GASCON assumed a 30 minute averaging time. Formulations were checked and adjusted to ensure that they reflect the 30 minute values. | Code change. |
| • Adjusted concentrations for event time in calculation of transient load. | Code change. |
| • Confirmation that the Von Karman constant should remain at 0.4. | No code change. |
| • Changes to the ground/elevated source criteria. If the source height is less than $(20 Z_o + 3)$ m than the ground formulations are invoked. | Code change. |
| • Changes to the virtual source formulations to ensure conservation of mass while equating the top-hat concentration to the plume centreline concentration. | Code change. |
| • Separating the drag zone from the air entrainment zone. | Code change. |
| • Revised "C" plane calculations, now SO ₂ cases are independent of geometry. | Code change. |
| • Information on CD2, a drag coefficient term. This term had significant impact on horizontal jets and it was recommended that it be set to zero. CD2 is now C _M , the added mass factor and is still an input parameter. | No code change. |

GASCON2 Changes Since July 1990 Evaluation

Impact on July Evaluation

Changes due to model review and running.

- | | |
|--|--|
| <ul style="list-style-type: none">• Changes to ground base cross-wind plume spreads.• Changed CD1, the jet expansion term. Now running at zero rather than 1.0. | <p>Code change: little impact.</p> <p>Input change: little impact.</p> |
|--|--|

If there was a code change there was likely some impact on the findings however, the changes were not always done one at a time. This made it difficult to determine the extent of any impact on a specific change. Only general comments in that regard can be made. Other minor model adjustments will likely continue to occur as we understand the findings from the field program better. For now, the above list captures the major changes that have been incorporated into the GASCON2 October 1990 model.

3 GASCON2 MODIFICATIONS AND INPUT FOR USE WITH SF₆

3.1 Model Modifications

The GASCON2 model was developed to estimate exposure zones from an uncontrolled sour gas release of H₂S or SO₂. However, the Field Measurement Program utilized sulphur hexafluoride (SF₆) as the tracer gas for the study. In order for comparisons to be made between field concentration data and GASCON2 concentration data, a modification to GASCON2 had to be implemented. This modification would allow GASCON2 to utilize nontoxic SF₆ as the dispersant instead of H₂S or SO₂.

For near surface (ground) plume releases, van Ulden's (1978) model was used to estimate crosswind integrated (CWI) ground level plume concentrations. The distribution of plume material in the crosswind direction is assumed to have a Gaussian or normal distribution. The vertical spread of the plume is assumed to follow the exponential form given by Horst (1979). With these assumptions, the ambient concentration is given by:

$$\chi(x, y, z) = \frac{0.73 f \dot{V}_{SF_6} (1.0 \cdot 10^{12})}{\sqrt{2\pi} U \sigma_Y \bar{Z}} \exp\left(-\frac{y^2}{2\sigma_Y^2}\right) \exp\left[-\left(\frac{z}{1.52\bar{Z}}\right)^2\right] \quad (3.1)$$

For unstable and neutral conditions, $\bar{Z}$ is not allowed to exceed the mixed layer height Z_i . For elevated plume releases, the frequently used Gaussian plume model is used (e.g. Turner, 1970). This model assumes that the distribution of plume material in the vertical and crosswind directions have a Gaussian or normal distribution. The ground level concentration is given by:

$$\chi(x, y, z) = \frac{f \dot{V}_{SF_6} (1.0 \cdot 10^{12})}{2\pi U_p \sigma_Y \sigma_Z} \exp\left(-\frac{y^2}{2\sigma_Y^2}\right) g \quad (3.2)$$

where: $\chi(x, y, z)$ = concentration of a given plume component (SF₆) at position (x, y, z) (ppt)

x = downwind distance from the rupture point (m)

y = crosswind distance (m)

z = height above ground level (m)

f = fraction of the plume remaining below the mixed layer height

$\dot{V}_{SF_6}$ = volumetric flow of the given plume component (SF₆) in the release (m³/s) at standard conditions

U_p = wind speed at plume height (m/s)

σ_Y = standard deviation of the plume in the crosswind direction (m)

σ_Z = standard deviation of the plume in the vertical direction (m)

Z_p = height of the plume above ground level (m)

$\overline{U}$ = mean transport wind speed for the plume (m/s)

$\overline{Z}$ = mean height to which the plume has dispersed (m)

g = function to account for vertical plume spread, depending on stability.

For stable unlimited mixing:

$$g = g_1$$

For unstable or neutral, plume trapping if $\sigma_z \leq 1.6Z_i$:

$$g = g_1 + g_2$$

For $\sigma_z > 1.6Z_i$:

$$g = g_3$$

where:

g_1 = function to account for plume reflections from ground

$$g_1 = \exp\left[\frac{-(z - Z_p)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z + Z_p)^2}{2\sigma_z^2}\right]$$

g_2 = function to account for plume reflections from inversion at mixed layer height Z_i if $\sigma_z \leq 1.6Z_i$

$$g_2 = \sum_{n=1}^N \left\{ \exp\left[\frac{-(z - Z_p - 2nZ_i)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z + Z_p - 2nZ_i)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z - Z_p + 2nZ_i)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z + Z_p + 2nZ_i)^2}{2\sigma_z^2}\right] \right\}$$

g_3 = function to account for uniform mixing of plume within mixed layer Z_i if $\sigma_z > 1.6Z_i$

$$g_3 = \sqrt{2\pi} \text{ and set } \sigma_z = Z_i$$

Note: $z = 0$ for Option 1-3 runs (June 1987 version; see Appendix A)
 $z = 1.5$ for final run and case studies (August 1990 version)

The z value was changed from zero to 1.5 m for the final runs and case studies because the sample probe inlet was located at a height of approximately 1.5 m above the ground. This change affects ground level releases but the affect on elevated is minimal. Therefore, caution should be exercised when comparing the Option 1-3 runs to the case studies and final runs.

$$\dot{V}_{SF_6} = \left(\frac{conv}{MW_{SF_6}} \right) (\dot{m}_{SF_6}) \left(\frac{P_{ST}}{P_{AMB}} \right) \left(\frac{T_{AMB}}{T_{ST}} \right) \quad (3.3)$$

Note: $\dot{V}_{SF_6}$ corrected to standard temperature and pressure (1 atm. and 0°C).

where:

$conv$ = conversion factor - volume of one kmole of a gas at 0°C and 1 atm. = 22.4 m³/kmole

MW_{SF_6} = molecular weight of sulphur hexafluoride = 146.06 kg/kmole

$\dot{m}_{SF_6}$ = mass flow rate of sulphur hexafluoride (kg/s)

P_{ST} = standard pressure = 101.3 kPa

P_{amb} = ambient pressure (kPa)

T_{ST} = standard temperature = 273 K

T_{amb} = ambient temperature (K)

3.2 Description of SF_6 Model Input Program

The large number of traverse files created a logistics problem because every file needed a corresponding model run. To facilitate this large number of GASCON2 model runs an input program was developed.

This program extracts input data from the integrated traverse files (Table 3.1) along with certain default parameters and sets up a GASCON2 input file for each traverse model run (Table 3.2). Each of the generated input files is then run through the GASCON2 model and a corresponding output file is created (Table 3.3).

3.2.1 Input Parameters

The GASCON2 input file format for a single model run is shown in Table 3.2. Approximately half of the inputs are defaults with the remaining data extracted from the integrated traverse files or from a meteorological file containing surface roughness, surface ambient temperature pressure. The meteorological data as well as the sulphur hexafluoride flow rates contained in the integrated traverse files have been travel time averaged. Travel time averaging involves averaging individual 3 minute data blocks over the time required for the plume to travel from the source to the analyser. This travel time is dependent on the wind speed and the distance to the arc. The surface ambient temperature and pressure are averaged over the test period while the surface roughness is a monthly average.

For this evaluation, GASCON2 will only use a minimum amount of field meteorological data as inputs. Surface heat flux, wind speed, ambient temperature, pressure, surface roughness and temperature gradient are the only field meteorological data parameters used. Other parameters such as Monin Obukhov length, surface friction velocity, mixing height, stability and σ_v and σ_w will all be generated internally in the model. Any model runs with missing field temperature gradient data were deleted from the evaluation.

The surface heat flux was generated from 10 m sonic anemometer data. If the surface heat flux term is missing from a traverse file, then the following calculation is applied:

$$H_o = (\rho_a) (C_{PA}) (W'T') \quad (3.4)$$

where:

H_o = surface heat flux (W/m²)

ρ_a = ambient air density at ground level ((kg/m³)

C_{PA} = specific heat of air at constant pressure (J/kg•K)

$W'T'$ = 10 m heat flux product (K•m/s)

Wind speed values used in the model were obtained from the 4 m sonic anemometer for ground releases and the 10 m sonic anemometer for elevated releases. The temperature difference found between the 25 m and 2 m levels comprised the temperature gradient. It should be noted that all of these meteorological inputs are obtained from the integrated traverse file and therefore, are travel time averaged.

The steady mass flow rate is given by:

Elevated Release:

$$\dot{m}_{air} = (U_{FAN}) (AE) (\rho_c) \left(\frac{P_c}{P_{amb}} \right) \left(\frac{T_{amb}}{T_c} \right) \quad (3.5)$$

where:

$\dot{m}_{air}$ = steady mass flow rate of air from the elevated source (kg/s)

U_{FAN} = fan velocity (m/s)

ρ_c = calibration air density (kg/m³) = 1.056 kg/m³

P_c = calibration pressure = 89.1 kPa

P_{amb} = surface ambient pressure (kPa)

T_{amb} = surface ambient temperature (K)

T_c = calibration temperature = 294.0 K

AE = fan cross-sectional area (m²)

Ground Release:

$$\dot{m}_{air} = (U_{FAN}) (AE) (\rho_C) \left(\frac{P_c}{P_{amb}} \right) \left(\frac{T_{amb}}{T_c} \right) \quad (3.6)$$

$\dot{m}_{air}$ = steady mass flow rate of air from the ground source (kg/s)

U_{FAN} = fan velocity = 2.36 m/s

ρ_C = calibration air density (kg/m³) = 1.056 kg/m³

P_c = calibration pressure = 94.4 kPa

P_{amb} = surface ambient pressure (kPa)

T_c = calibration temperature = 294.0 K

T_{amb} = surface ambient temperature (K)

AE = fan cross-sectional area (m²)

Table 3.1
Integrated Traverse Data File Format

Field	Variable	Unit
1	Field Test	1 to 33
2	Analyser ^(a)	1, 2 or 3
3	Traverse Number	
4	Month	10, 11 or 12
5	Day	1 to 31
6	Year	1988
7	Start Hour	0 to 23
8	Start Minute	0 to 59
9	Start Second	0 to 59
10	Finish Hour	0 to 23
11	Finish Minute	0 to 59
12	Finish Second	0 to 59
13	Arc Code ^(b)	1 to 5
14	Source Code ^(c)	1 to 5
15	Distance (m)	700, 1400 or 2100
16	Number of Time Intervals	
17	Release Height Code ^(d)	6 or 7
18	SF ₆ Release Rate	(g/min)
19	Fan Velocity	(m/s)
20	Moment Method	
21	Sigma y	(m)
22	Mean Absolute Percentage	
23	Mean Absolute Residual Concentration	(ppt)
24	Maximum Concentration	(ppt)
	Centroid Position	(m)
25 to 29	Same as 20 to 24 for Hanna Method	
30 to 34	Same as 20 to 24 for Concentration Maximum Method	
35	Crosswind Integrated Concentration	(ppt m)
36	Skewness	
37	Kurtosis	
38	Transport Angle	(degrees)
39	Easting Coordinate	(m)
40	Northing Coordinate	(m)
41	4 m Sonic Data	
42	Counts	
43	Wind Speed	(m/s)
44	Wind Direction	(degrees)
	$\overline{U^2}$	(m/s) ²

Table 3.1 (Continued)
Integrated Traverse Data File Format

Field	Variable	Unit
	4 m Sonic Data	
45	$\overline{V'^2}$	(m/s) ²
46	$\overline{W'^2}$	(m/s) ²
47	$\overline{W'T'}$	(m K/s)
48	$\overline{U'W'}$	(m/s) ²
49	H_o	(W/m ²)
50	U^*	(m/s)
51	L	(m)
52	Z/L	
53	σ_θ	(degrees)
54	σ_w	(m/s)
55	σ_ϕ	(degrees)
56 to 70	Same as 41 to 55 for 10 m Sonic Data	
71	Ambient Temperature	(°C)
72	$T_{25} - T_{16}$	(°C)
73	$T_{16} - T_{10}$	(°C)
74	$T_{10} - T_2$	(°C)
75	Incoming Radiation	(W/m ²)
76	Outgoing Radiation	(W/m ²)
77	Net Radiation	(W/m ²)
78	Soil Heat Flux	(W/m ²)
79	Mixing Height	(m)

^(a)Analyser Code

1 = Analyser A
2 = Analyser B
3 = Analyser C

^(b)Arc Code

1 = Centre Sampling Circle
2 = North Sampling Arcs
3 = East Sampling Arcs
4 = South Sampling Arcs
5 = West Sampling Arcs

^(c)Source Code

1 = Centre Source Location
2 = North Source Location
3 = East Source Location
4 = South Source Location
5 = West Source Location

^(d)Release Height Code

6 = Surface Release
7 = Elevated Release

Table 3.2
SF₆ Program Input File Parameters

Term	Description	Units	Default
Trans	Transient run indicator	-	N
Ignite	Ignited case indicator	-	N
Risk	Output risk data?	-	N
Rise	Output plume rise data?	-	Y
Concn	Output concentration data?	-	Y
Summary	Output summary data	-	Y
Conc 1	Hazard zone for 3-minute average concentration	ppt	1000.00
Conc 2	Hazard zone for 3-minute average concentration	ppt	3000.00
Conc 3	Hazard zone for 60-minute average concentration	ppt	2000.00
Conc 4	Hazard zone for 60-minute average concentration	ppt	1000.00
TAVG 1	Time average constant # 1	minutes	3.00
TAVG 2	Time average constant # 2	minutes	3.00
TAVG 3	Time average constant # 3	minutes	60.00
TAVG 4	Time average constant # 4	minutes	60.00
IYR	Year	-	-
IMON	Month	-	-
IDAY	Day	-	-
IHOURL	Hour	-	-
EQ DIA	Diameter of source	mm	2195.2 for ground 737.0 for elevated
Mesdy	Steady mass flow rate from the source	kg/s	-
LAMBDA	Release angle from horizontal	degrees	90.0
ZINIO	Exit height of source above ground	m	0.40 for ground 2.31 for elevated
Fedge	Minimum plume remaining in mixed layer	-	0.05
CDOT	Plume volumetric source/sink term	kg/s	0.00

Table 3.2 (Continued)

Input Deck

Term	Description	Units	Default
QDOT	Plume volumetric source/sink energy term	W/m ²	0.00
VFH ₂ S	Volume fraction of H ₂ S in gas	-	0.00
VFCH ₄	Volume fraction of methane in gas	-	0.00
QHP	Lower heating value of gas (air)	-	0.00
CPE	Specific heat at constant pressure (air)	J/kg·K	1005.0
MWGAS	Molecular weight of gas (air)	kg/mole	28.967
TI	Exit temperature of gas from source	°C	-
SF _g	Steady release rate of SF ₆	g/min	-
Uref	Surface reference wind speed	m/s	-
Zref	Surface reference height for wind speed	m	-
TaO	Surface ambient temperature	°C	-
PaO	Surface ambient pressure	kPa	-
ZZO	Surface roughness	m	-
ZZ1	Mixing height	m	-
LAT	Latitude of site	degrees	51.00
Ho	Surface heat flux	W/m ²	-
TTGRA	Temperature gradient (2-25 m)	K/m	-
L	Monin-Obukhov length	m	-
WSIar	Convective velocity scale	m/s	-
USIar	Surface friction velocity	m/s	-
Sigma V	Cross wind sigma	m/s	-
Sigma W	Vertical wind sigma	m/s	-

Table 3.3

SF₆ Model Output Summary for Each Traverse

1.	Test Number
2.	Analyser Number
3.	Traverse Number
4.	Month
5.	Day
6.	Hour (start)
7.	Minute (start)
8.	ARC Radius
9.	SF ₆ Flow Rate (g/min)
10.	Fan Velocity (m/s)
11.	Steady Mass Flow Rate (kg/s)
12.	Reference Wind Speed (m/s)
13.	Reference Height (m)
14.	Ambient Temperature (°C)
15.	Ambient Pressure (kPa)
16.	Surface Roughness (m)
17.	Mixing Layer Height (m) - (input)
18.	Surface Heat Flux (W/m ²) - (input)
19.	Atmospheric Stability - model
20.	Ambient Temperature Gradient (°C/m) - (input)
21.	Monin-Obukhov Length (m) - (input)
22.	Convective Velocity Scale (m/s) - (input)
23.	Surface Friction Velocity (m/s) - (input)
24.	Sigma V (degrees) - (input)
25.	Sigma W (degrees) - (input)
26.	Ambient Air Density (kg/m ³)
27.	Power in Irwin Power-law Model
28.	Ambient Temperature Gradient (°C/m) - (model)
29.	Monin-Obukhov Length (m) - (model)
30.	Convective Velocity Scale (m/s) - (model)
31.	Surface Friction Velocity Scale (m/s) - (model)
32.	Mixing Layer Height (m) - (model)
33.	Briggs Momentum Plume Rise (m)
34.	Briggs Buoyancy Plume Rise (m)
35.	Stable Calm Plume Rise (m)
36.	Sum of Cubes Plume Rise (m)
37.	Briggs Final Plume Rise (m)
38.	Integral Plume Rise (m)
39.	Zp Plume Rise (m)
40.	Ground Level Concentration (3 min) - ppt
41.	Sigma Y (m)
42.	Sigma Z (m)
43.	STD SGY (m)
44.	STD SGZ (m)
45.	Stability Source Indicator
46.	Sigma Y (m) - moment
47.	Maximum Concentration (ppt) - moment
48.	Sigma Y (m) - hanna
49.	Maximum Concentration (ppt) - hanna
50.	Sigma Y (m) - Concentration Max.
51.	Maximum Concentration (ppt) - Concentration Max.
52.	Skewness
53.	Kurtosis
54.	Sigma U (m/s)
55.	Sigma V (m/s)
56.	Sigma W (m/s)
57.	Sigma Theta (degrees)
58.	Sigma Phi (degrees)
59.	Z/L

4 GASCON2 MODEL EVALUATION

4.1 Introduction

Evaluations of any model usually focus on determining the accuracy of model predictions compared to actual observations. Since dispersion models are frequently used for decision making with respect to a facility operation, it is important that some level of confidence be associated with the model. The results of various comparisons of GASCON2 model predictions with tracer dispersion data collected during the Field Measurement Program are presented in this section.

In recent years, considerable effort has been put forth on determining performance measures for dispersion models (Hanna, 1985; Cox, 1988). A wide variety of performance indices have been suggested since it is difficult to arrive at a single quantitative index of accuracy. As there are strengths and weaknesses associated with each method, several different techniques have been included in this evaluation. These performance techniques can be measured on data sets that contain predicted and observed values that are either paired or unpaired in time and/or space.

Pairing the predicted and observed values may be useful if a large data set is available and an understanding of the model's behavior is desired. The performance of the model can be related to individual meteorological inputs.

Comparisons of predicted and observed values that are unpaired in time and space are of particular use when exactly matching meteorological data inputs are not available or are uncertain, and when the primary goal of the evaluation is to determine the ability of the model to predict the maximum concentrations that may occur. The protocol established by the United States Environmental Protection Agency (EPA) for screening and testing a model for use in regulatory analysis was developed for unpaired data (Cox, 1988).

One other consideration that was unique to the FMP data set was the fact that most models use time-averaged plume dispersion coefficients based on a composite value (meander plus relative dispersion). This evaluation's protocols were established based on this premise, however, the data collected in the Field Measurement Program was instantaneous (1 to 30 second average). This difference in averaging times should be considered in any model evaluation and are discussed further in Section 4.4.4.

4.2 Data Base Quality Assurance

4.2.1 Data Base Screening

A review of the tracer data base was conducted to assess its quality and suitability for use in the model evaluation. First, the Gaussian approximations made using the Moment method were examined. Sixty-six (approximately 7%) of the traverse profiles were not well represented by this fit. An additional 3% of the traverses were conducted after the source had been turned off for the purposes of determining plume decay rates. These traverses introduced some additional uncertainty into the evaluation results.

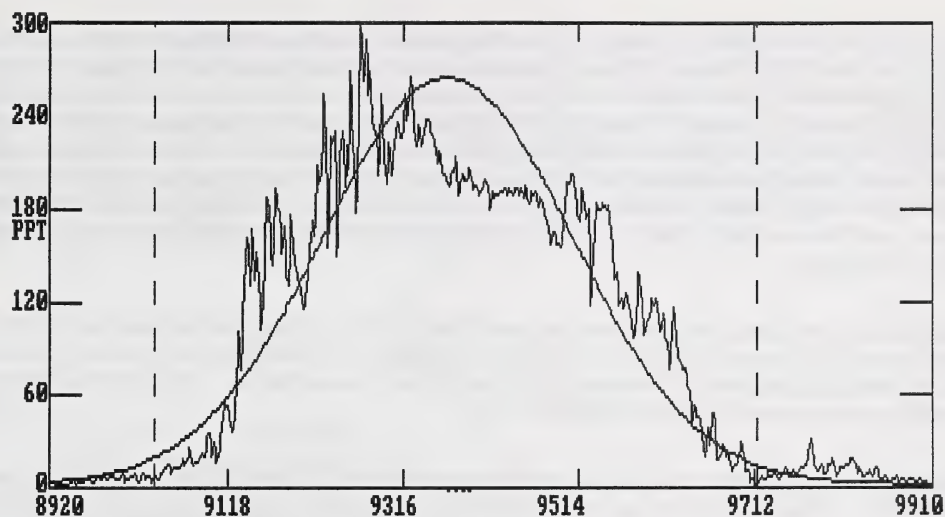
4.2.2 Angle of Traverse Effects

One **important** uncertainty in the tracer data base was the potential for a traverse to cross the plume centreline at an angle of intersection of less than 90 degrees. As long as the vehicle crosses the plume centreline, the maximum concentration should be accurate (except for a slight correction in downwind difference). As the angle of intersection is reduced the apparent observed plume dispersion coefficients (σ_y) increases. The error is a function of the angle of the traverse to the centreline and to a lesser extent the plume width itself. Table 4.1 shows the magnitude of the error as the angle of the traverse deviates away from a perpendicular intersection with the plume centerline. Although this is an **important** uncertainty, the angle deviation can be as great as 60 degrees before the error in the observed σ_y reaches a factor of two, and the maximum concentrations are relatively unaffected.

A further consideration in the use of the tracer data base was the existence of traverses which were made parallel to the plume centreline and consequently never cross the centreline. An example is shown in Figure 4.1. The broad flat peak results from the analyser following a relatively constant concentration path parallel to the centreline. The amplified concentration fluctuations are a consequence of increased mixing in the edges of the plume. Often a large and unrealistic σ_y value results from the extended longitudinal path through the plume. Additionally, the observed maximum concentration does not reflect the true maximum, since the centreline concentration is never measured. Although many of these parallel traverses can be identified, not all are obvious. Consequently, they have not been screened from the data set. Therefore, data in the lower concentration ranges should be treated with caution, since these observations may indicate a lower maximum concentration than actually existed.

Table 4.1
Angle of Traverse Effects

Angle (degrees)	Error (%)
0	0
10	2
15	4
30	15
45	41
60	100
70	192
75	286
80	476
85	1047
88	2765
90	∞



TRAVERSE STATISTICS (T12C28)

File scans: data (50 to 450), moment (128 to 407)

Date: 11-18-1988 Time: 22:27:40 to 22:34:20

Start location: Z1 on 2100 m South arc Source: South

Power law calibration:

Time = 16.72,

$$\text{ppt} = 1181.6 \cdot (\text{voltage})^{1.3271}$$

$$\text{For volt} > .7105: \text{ppt} = 1037.7 \cdot (\text{voltage})^{.9472}$$

Time = 27.33,

$$\text{ppt} = 723.9 \cdot (\text{voltage})^{1.1179}$$

$$\text{For volt} > 2.938: \text{ppt} = 771.6 \cdot (\text{voltage})^{1.0587}$$

Method	Sigma Y (m)	Mean Abs. Res (%)	Mean Abs. Res (ppt)	Max. Conc. (ppt)	Plume Center on arc (m)
Moment	141.5	23.59	36.41	265	9366.4
Hanna	161.1	18.80	27.51	237	9364.6
Maximum	127.9	59.21	74.50	299	9268.0

CW int. conc. (ppt m): 95846.92, % in moment: 98.07

Skewness: 0.162

Kurtosis: 2.13

Centroid location: (North 3123.4 m, East 834.3 m)

Transport from 184.53 degrees

Figure 4.1

Example of Analyser Traverse Parallel to Plume Centerline.

4.2.3 Uncertainties in Meteorological Inputs and Time Averages

In considering the performance of a model designed to estimate short term concentrations such as GASCON2, it should be remembered that typical model evaluations involve averaging times of at least one hour. Special considerations are involved for three minute averaging periods, especially when compared to real time plume data during low wind speed, stable conditions. For instance, even though the displacement of the meteorological data tower from the tracer receptors and the tracer release was included in pairing traverse data with meteorological data, the long travel times between the meteorological tower, the tracer source, and the analyser vehicles under low wind speeds introduces significant uncertainty in this matching.

Additionally, tracking the plume may be particularly difficult due to plume meander at low wind speeds. This results both in fewer data points under the conditions of greatest interest and in traverses that may not represent true centreline concentrations. The effects of these parallel traverses are discussed in Section 4.2.2.

Both paired and unpaired analyses of predicted and observed concentrations were used for this model evaluation. However, the comparison of predicted and observed values paired in time and space may provide an unrealistic measure of the model's performance. Model inputs may be incorrectly specified due to mismatched meteorological data, while traverses parallel to the centreline may indicate lower than actual concentrations. Other evaluations of model predictions usually involve longer averaging times which reduce many of these discrepancies. Consequently, an unpaired analysis of the data takes on greater importance for this evaluation.

Another critical factor in this model evaluation is the difference in averaging times between the model predictions and observed plume concentrations. GASCON2 generates three minute average concentrations, while the data from the Field Measurement Program provides essentially instantaneous (1 to 30 second average) maximum concentrations. Instantaneous centreline concentrations will be higher than time averaged values due to the effects of plume meander, so the three minute average concentrations predicted by GASCON2 should underpredict the instantaneous concentrations from the field data. This uncertainty is discussed further in Section 4.4.4.

4.2.4 Effects of Analyser Response Time

When concentration data are collected in real time, the potential effects of the analyser response time on the data set should be considered. If concentration fluctuations occur at much faster rate than the analyser can measure, peak concentrations may be attenuated by the system; i.e. measured values may be lower than the actual values. The response time of each analyser system was measured by injecting a standard gas with a known concentration of tracer into the air sampling inlet and measuring the time required for the analyser signal to rise to 63% of its final response. The effects of the system response time can then be calculated as follows:

$$\frac{C_m}{C_a} = 1 - e^{-\frac{t}{\tau}} \quad (4.1)$$

where

C_a = actual concentration

C_m = measured concentration

t = duration of concentration C_a

τ = analyser system response time.

The results of this calculation for the FMP analyser system response time of 1 second are plotted in Figure 4.2. This curve represents the attenuation in signal for concentration fluctuations of different time scales. Concentration changes with a two second duration register 86% of the actual change. Peaks with a three second duration would be measured at 95% of their actual concentration. Plume concentration fluctuations were not significant at faster time scales than these, so the analyser system response time was sufficiently fast enough to measure the peak concentrations that occurred during the field measurement program.

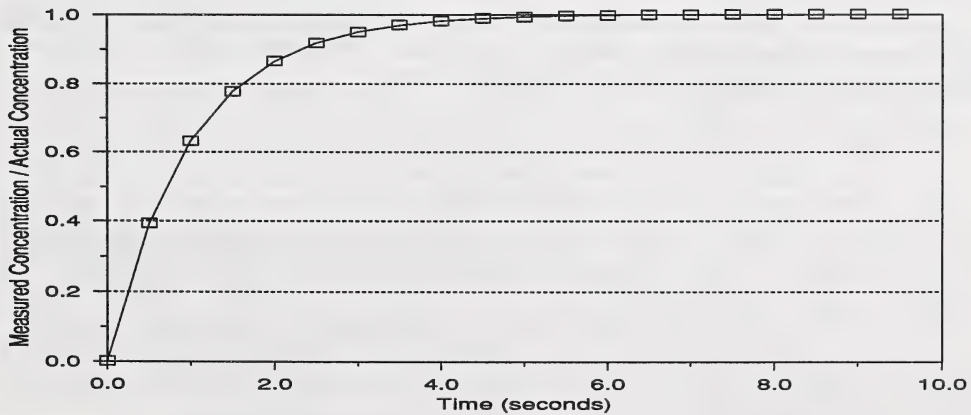


Figure 4.2

Attenuation of Analyser Response as a Function of Concentration Fluctuation Time Scales for a System Response Time of 1 Second.

4.3 Model Evaluation Techniques

4.3.1 Factor of Two Analysis

The EPA (Cox, 1988) has stated that a factor of two is a reasonable performance target for a model to achieve before it is used for refined regulatory analysis. The premise of that requirement is based on observations typically on the order of 30 minutes to 1 hour or more. We assume that the factor of two requirement specifies that the model will predict within a factor of two for unpaired data 100% of the time. It is not certain whether the EPA would consider this to be a requirement for model comparisons using three minute averages or instantaneous data.

4.3.2 Statistical Analysis

Hanna (1985) proposed a single dimensionless mean square error, M , as a unique measure of model performance. M is a function of several other standard statistical measures. Hanna recommended a paired data analysis for large data sets.

The EPA (Cox, 1988) protocol document for determining the best performing model identifies a screening test based on fractional bias for the highest 25 unpaired cases and includes test statistics, a composite performance measure and also a standard error determination.

To cover the range of required statistics recommended by both Hanna and the EPA, the following statistical values were calculated:

Correlation Coefficient

A correlation is a quantitative measure of agreement between predicted and observed values. The Pearson product-moment correlation coefficient is frequently used and assumes a linearity between predicted (P) and observed (O) values:

$$r = \frac{\sum(O - \bar{O})(P - \bar{P})}{\sqrt{\sum(O - \bar{O})^2 \sum(P - \bar{P})^2}} \quad (4.2)$$

The correlation coefficient can be represented visually by scatter plots of predicted and observed values. In spite of model improvements, deviations between predictions and observations are still relatively large due to inherent uncertainties. For this reason, correlation coefficients should only be used as a relative rather than absolute measure of model performance. For example, in a recent EPRI model development project, an improved model resulted in a r^2 of 0.34, a significant improvement over the CRSTER model ($r^2 = 0.02$) (Venkatram 1988).

Residuals Analysis

The residual or difference is defined as :

$$d = O - P \quad (4.3)$$

and the associated residual statistics are given below. The mean of the difference

$$\bar{d} = \frac{\sum d}{N} \quad (4.4)$$

is referred to as the bias. The bias indicates whether the model generally over or under predicts. For a normally distributed variable, the bias is also normally distributed. The variance of the difference is given by

$$S_d^2 = \frac{\sum (d - \bar{d})^2}{N - 1} \quad (4.5)$$

and is a measure of the average spread of the difference (noise). For a normally distributed variable, the variance has a chi-squared distribution.

Hanna's proposed M is really a mean square error term defined as:

$$\text{Hanna's } M = \frac{MSE}{(\bar{P} \bar{O})} = \frac{\overline{(P - O)^2}}{(\bar{P} \bar{O})} \quad (4.6)$$

where $MSE = \text{Mean Square Error}$

The MSE provides a measure of the gross variability. The mean square error has a compound distribution. Again, it must be emphasized that these residual statistics, like the correlation coefficients, can only provide a relative, rather than absolute, performance statistic. In the application of these performer statistics, the performance should be applied to a reference model as well as to the model under review. A low value of M indicates a better model. This procedure automatically weights higher concentrations more, because the difference $(P - O)$ is likely to be largest at highest concentrations.

Two other measures of paired data error have been used:

$$\text{Relative Mean Absolute Error} = \text{RMAE} = \frac{1/N \sum |O - P|}{\bar{O}} \quad (4.7)$$

and

$$\text{Mean Relative Absolute Error} = \text{MRE} = \left\{ \frac{2}{N} \sum_{i=1}^N \left(\frac{[P_i - O_i]}{[P_i + O_i]} \right)^2 \right\}^{1/2} \quad (4.8)$$

Fractional Bias

Fractional bias can be used to compare predicted and observed values that are either paired or unpaired in time and space. Irwin (1983) used the fractional bias to help evaluate plume dispersion coefficients. The fractional bias is defined by:

$$\text{Fractional Bias} = FB = \frac{2(\overline{O} - \overline{P})}{(\overline{O} + \overline{P})} \quad (4.9)$$

The fractional error has the property of being logarithmically unbiased, having the same numerical value (although different signs) for an overestimate of N times the observed value or for an underestimate of $1/N$ times the observed.

Calculation of fractional errors has also been suggested by the EPA for unpaired data, where $\overline{O}$ and $\overline{P}$ refer to the average of the observed and predicted highest 25 values.

The fractional bias may be used as screening test. Models that pass the screening test are then subjected to a more comprehensive statistical comparison. First a test statistic is used to compare the performance by computing a robust estimate of the highest concentration (RHC). Second, a composite performance measure is computed for the model as a weighted linear combination of the individual fractional bias components. And third, a standard error determination is made.

To help evaluate how a model works, residuals should be plotted against important model inputs (such as wind speed and plume dispersion coefficients). Ideally, the residual should be uniformly distributed about zero over the whole range of the model input. Any significant departure from zero over the range might indicate a problem with the physics in the model.

4.4 Model Evaluation Results

4.4.1 Paired Analysis

The three-minute average concentrations predicted by GASCON2 were compared to the instantaneous concentrations determined by the moment method and maximum concentration method fits of the observed data described in Volume 1 of the FMP report series. (By definition, the maximum concentration method reports the maximum concentration observed during a traverse.) In this section, the results of comparison statistics generated for predicted and observed concentrations paired in time and space are presented. Final run statistics for ground and elevated cases using GASCON2 are shown in Table 4.2. Comparisons in this table are for both the moment method and maximum concentration method. However, only the moment method results are discussed below.

Table 4.2

Detailed GASCON2 Statistics - All Cases

	MEAN $\frac{P}{O}$	MEDIAN $\frac{P}{O}$	MEAN $\frac{O}{P}$	MEAN $\frac{P}{O}$	MEAN $\frac{O}{P}$	MEDIAN $\frac{P}{O}$	MEDIAN $\frac{O}{P}$	MEDIAN $\frac{P}{O}$	MEDIAN $\frac{O}{P}$	RMAE	HANNA'S M	SLOPE	INTERCEPT	AVG. BIAS	MRE	% WITHIN FACTOR OF 2	% WITHIN FACTOR OF 3
FINAL RUN Moment Maximum (Ground)	4.350 3.028	0.444 0.396	2057.6 2482.3	1183.6 1183.6	0.575 0.477	1798.5 2109.0	599.1 599.1	0.333 0.284	0.170 0.139	0.954 0.917	3.100 3.386	-0.160 -0.115	1565.6 1522.8	874.0 1298.7	0.860 0.876	23.0 29.4	36.6 45.3
FINAL RUN Moment Maximum (Elevated)	5.128 3.551	1.441 1.273	768.4 897.6	1234.9 1234.9	1.607 1.376	583.0 688.5	707.4 707.4	1.213 1.027	0.281 0.250	1.273 1.108	3.434 3.030	0.618 0.467	762.9 824.4	-466.5 -337.3	0.718 0.694	39.7 42.0	65.5 68.0

Factor of Two Analysis

The factor of two analysis is presented graphically in Figure 4.3. Ratios of predicted to observed concentrations were scaled using a base two logarithm to provide increments of a factor of two. For instance, if $\log_2(P/O) = 1$, then $P/O = 2$, and the overprediction is a factor of two. A value of $\log_2(P/O) = 2$ equates to an overprediction by a factor of four. Positive values represent overprediction and negative values represent underprediction. Twenty-three percent of the predicted concentrations for ground release cases were within a factor of two of the observed concentrations, while 40 % of the elevated case predictions were within a factor of two of the observed concentrations.

As indicated by the top two graphs in Figure 4.3, both the ground and elevated data sets indicate both over- and underpredictions ranging from 0 to greater than factors of 30. In general, the predictions for the ground releases have a greater tendency to underpredict the observed concentrations more often than the elevated releases. This is further shown by the histograms in Figure 4.3. Over 45% of the ground release predictions underpredict the observed concentrations by greater than a factor of three, while less than 10% of the elevated case predictions fall in this range. Approximately 17% of the ground release predictions overpredict the observed concentrations by greater than a factor of three, while approximately 25% of the elevated predictions exceed the observed values by greater than a factor of three.

Correlation Coefficient

Scatter diagrams of the predicted and observed concentrations for both ground and elevated releases are shown in Figure 4.4. Predicted concentrations were plotted versus observed field data for all available cases. The correlation coefficient (r) for the ground release cases was 0.17 and for elevated release cases was 0.28.

The meteorological preprocessor used to convert the meteorological data into a form useable by GASCON2 classified some stable conditions observed in the field program as neutral, and vice versa. To address this uncertainty, Figure 4.5 shows scatter plots of predicted and observed concentrations only for runs which the preprocessor classified as stable. The correlation coefficient for the ground release predictions using only stable classifications was 0.13; for elevated releases it was 0.19. Since these correlation coefficients are worse than those for the correlations of all stability classes, there does not appear to be any value to examining runs classified as stable by the model as opposed to all runs. This may be due in part to neutral conditions which were mistakenly classified as stable.

Residuals Analysis

The results for the residuals analysis discussed in Section 4.3.2 are also listed in Table 4.2. The average bias for ground releases was 1298, indicating general underprediction, while the average bias for elevated releases was -337, indicating general overprediction. This is consistent with the factor of two analyses discussed earlier. Values of Hannah's M , relative mean absolute error, and mean relative error are also tabulated in Table 4.2.

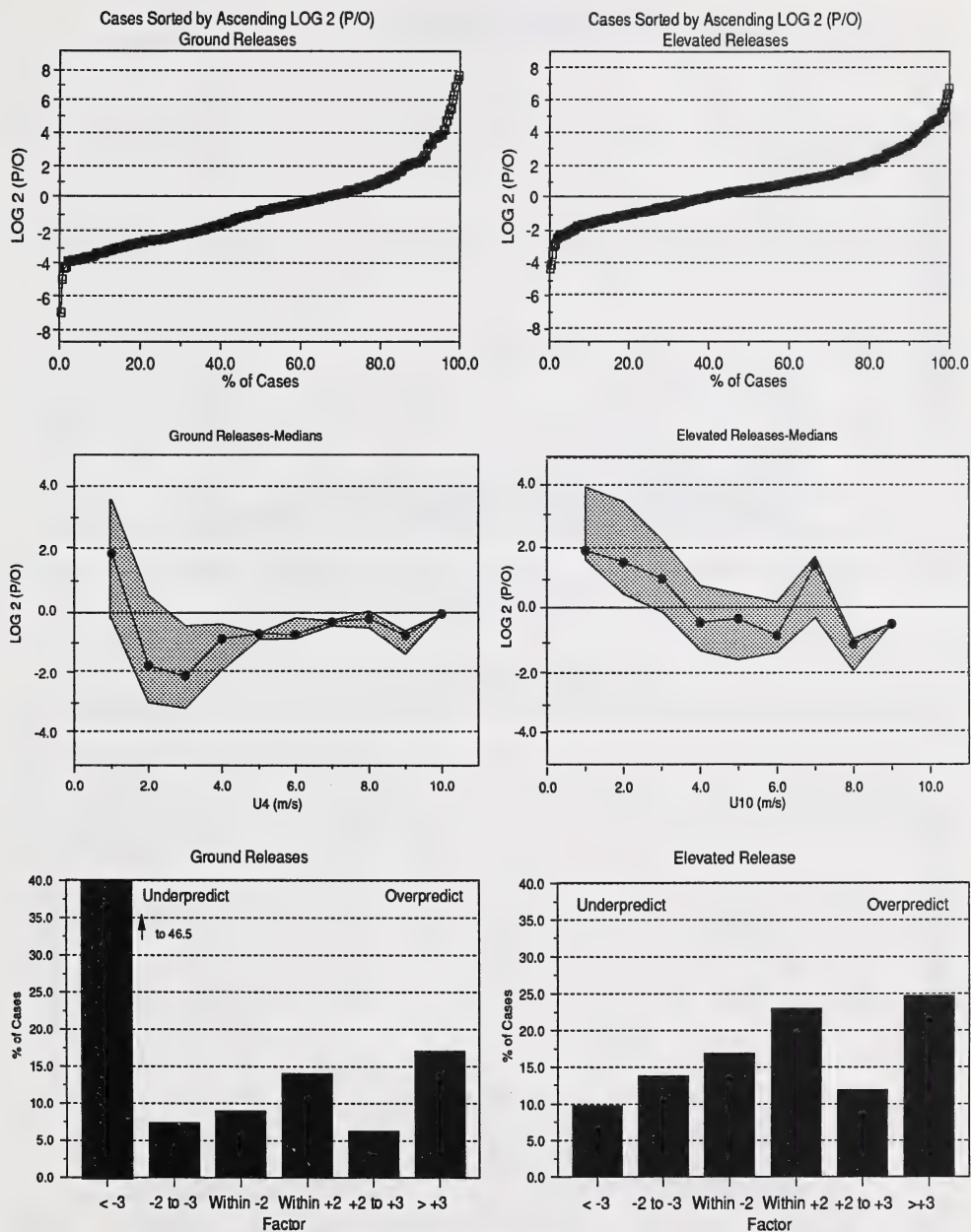


Figure 4.3

Comparisons of Paired GASCON2 Model Predictions and Observed Concentrations for Ground and Elevated Releases.

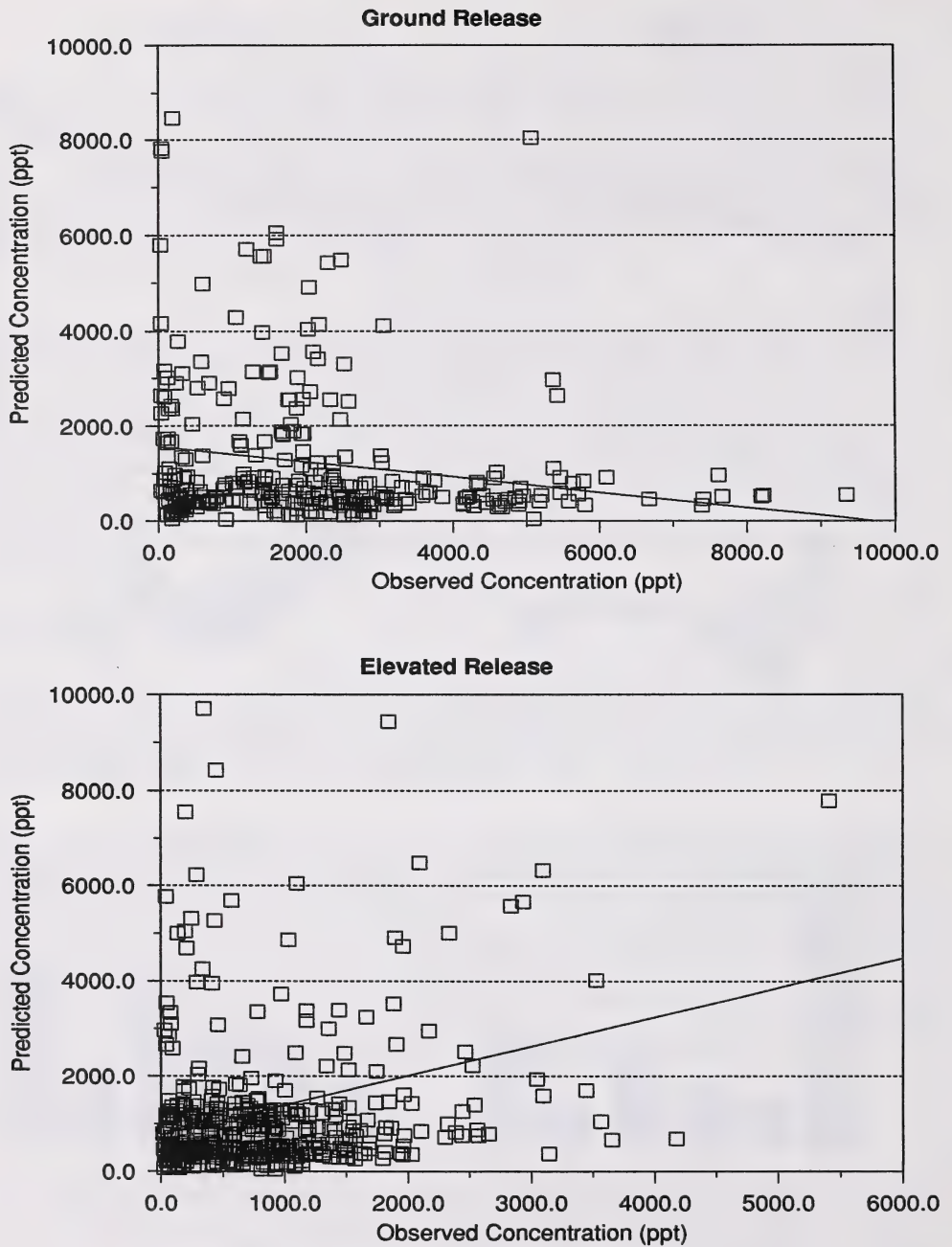


Figure 4.4

Scatter Diagrams of Paired GASCON2 Model Predictions and Observed Concentrations for all Stability Classes of Ground and Elevated Releases.

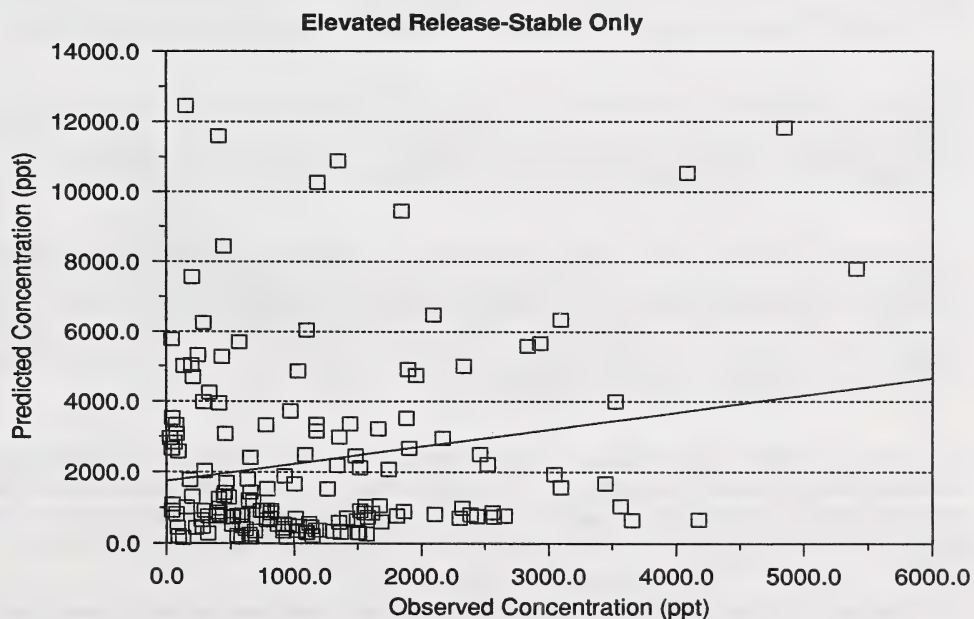
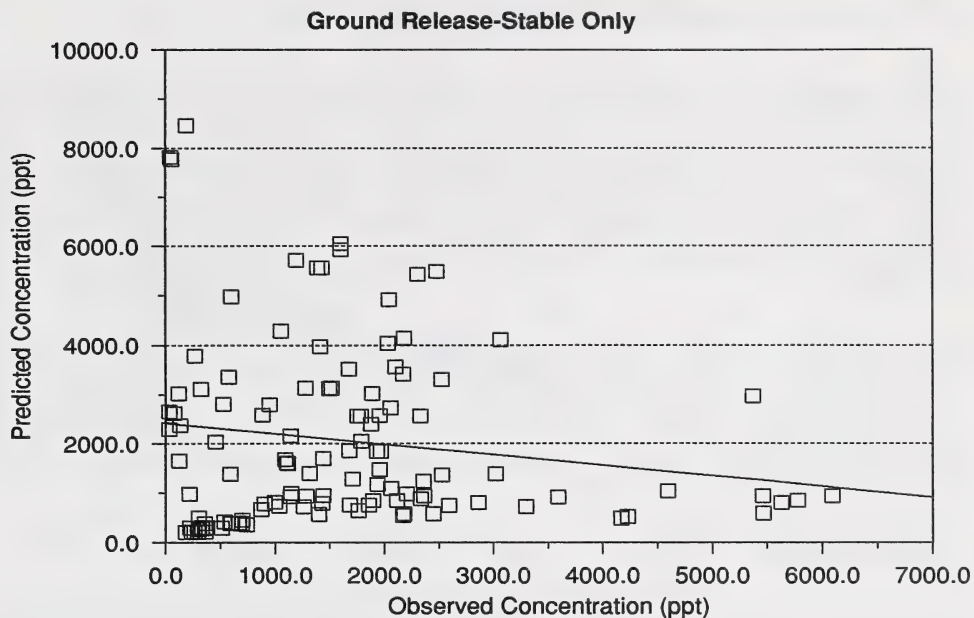


Figure 4.5

Scatter Diagrams of Paired GASCON2 Model Predictions and Observed Concentrations for Cases Labeled Stable by the Meteorological Preprocessor for Ground and Elevated Releases.

Performance Ranked by Normalized Concentration

For emergency response and air toxic risk assessments, the primary concern is the estimation of the worst case concentrations that may occur during a given release scenario. To determine the worst case conditions in the tracer data base, the observed concentrations were normalized by dividing by the tracer release rate (C/Q). Comparisons of dispersion can then be made between all tests, even though the release rate varied from period to period. High values of C/Q indicate low dilution of the tracer release from the source. By sorting the data base by increasing values of C/Q , the worst case conditions of low dilution are easily identified.

Figure 4.6 presents graphs of base 2 logarithms of the ratio of predicted to observed paired concentrations, sorted by increasing values of C/Q . These graphs indicate a trend of increasing underprediction by the model with increasing normalized concentration for both ground and elevated releases. Consequently the model tends to underpredict during the worst case concentration periods. This tendency may be influenced by uncertain matching of meteorological inputs to the model.

4.4.2 Unpaired Analysis

As indicated previously, the primary concern for emergency response and air toxic risk assessments is the estimation of the worst case concentrations that may occur during a given release scenario. If a model can predict the highest range of concentrations that may result from a release, its ability to determine the exact time and place of the occurrence is secondary.

Worst case conditions in the tracer data base were determined as described above by normalizing the observed tracer concentrations by the tracer release rate. Large values of normalized concentration (C/Q) indicate low dilution of the tracer release; these are the conditions that would produce the highest concentrations in a toxic release scenario.

To evaluate GASCON2 using unpaired predicted and observed values, the same model predictions that were generated for the paired evaluation were used. In Figure 4.7, the predicted and observed values of all ground releases at the downwind arc distances of 700 and 1400 m have been sorted independently by increasing C/Q values. In general, GASCON2 underpredicts the observed concentrations. However, in the region of higher C/Q values, the model does follow the trend of the increasing concentrations.

The results for the elevated releases at the 700 m and 1400 m arcs exhibit a somewhat different trend, as shown in Figure 4.8. The predictions for the elevated releases at the 700 m arc uniformly overpredict the observed concentrations, but again follow the correct trend. At the 1400 m arc, there is general underprediction in the region of higher C/Q values.

The fractional bias can be calculated to quantify the general observations made from Figures 4.7 and 4.8. A common model evaluation technique uses the fractional bias of an arbitrary number of the highest unpaired predicted and observed values, such as the top 10% or the top 25 values. Since the goal of this evaluation is to determine model performance under worst case conditions, the ranges of values selected for this analysis were determined by inspection of Figures 4.6 and 4.7. The critical regions were selected using changes in the slope of the observed normalized concentration curve. The results of the fractional bias calculations for the both average and standard deviation are listed in Table 4.3

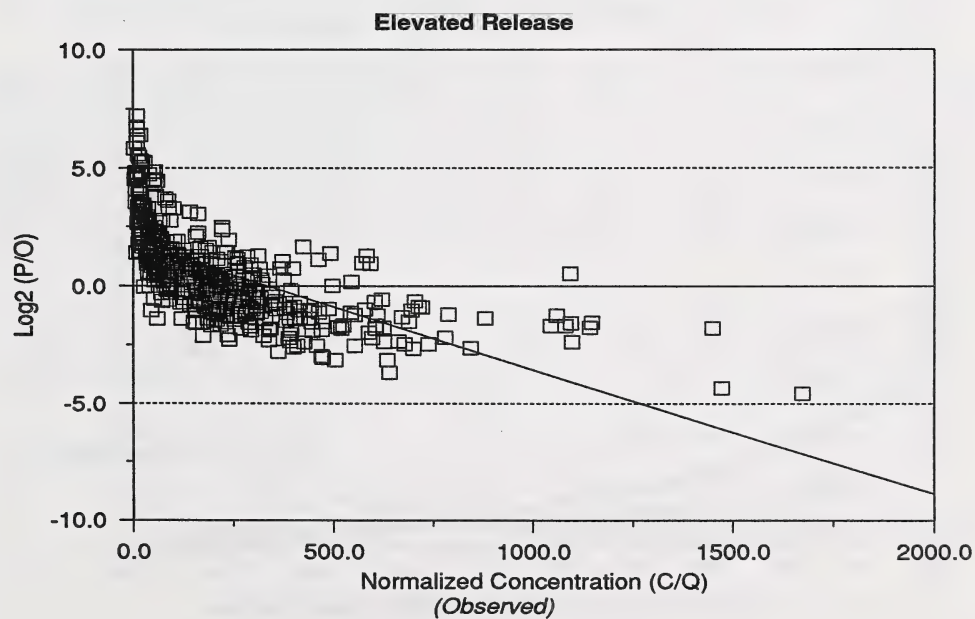
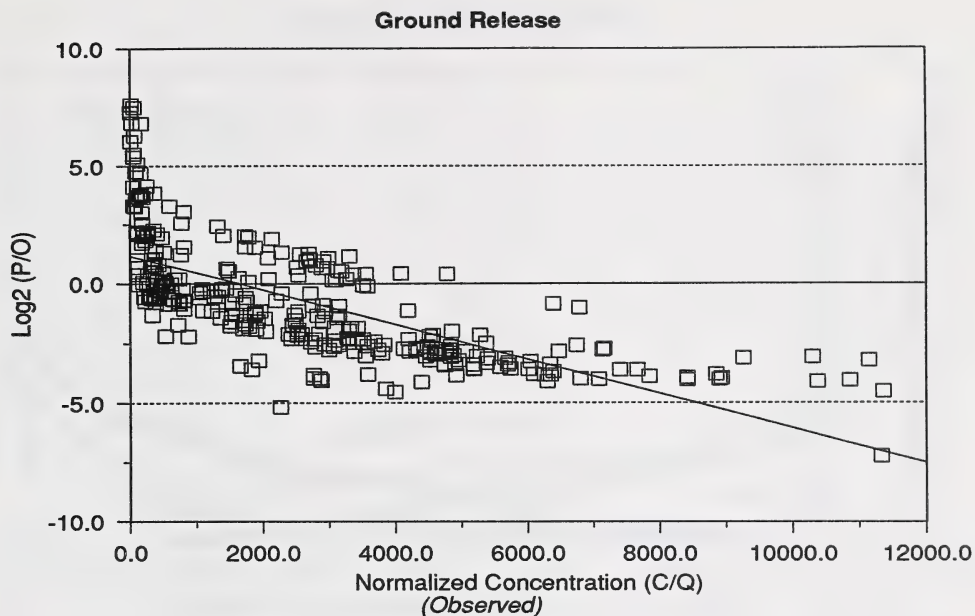


Figure 4.6

**Comparisons of Paired GASCON2 Model Predictions and Observed Concentrations
Sorted by Observed Normalized Concentration for Ground and Elevated Releases.**

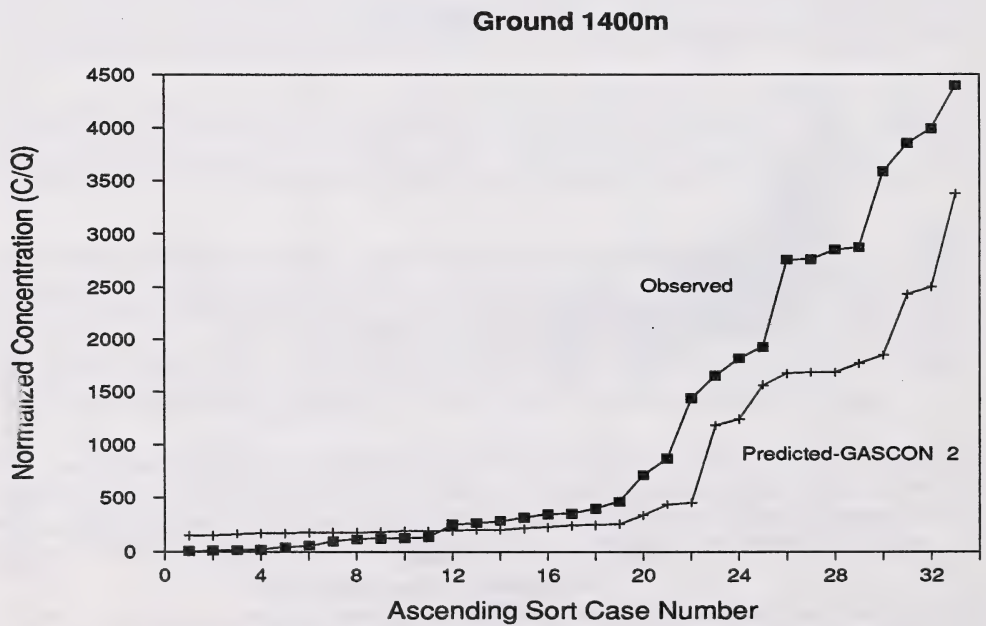
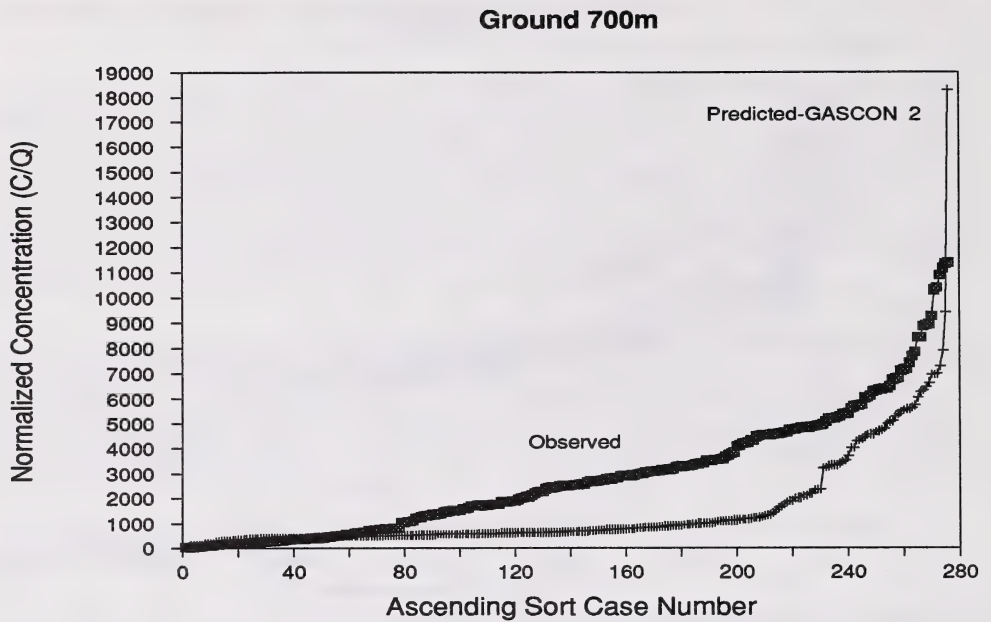


Figure 4.7

Unpaired GASCON2 Model Predictions and Observed Concentrations for Ground Releases Normalized by Tracer Release Rate and Sorted Independently by Normalized Concentration.

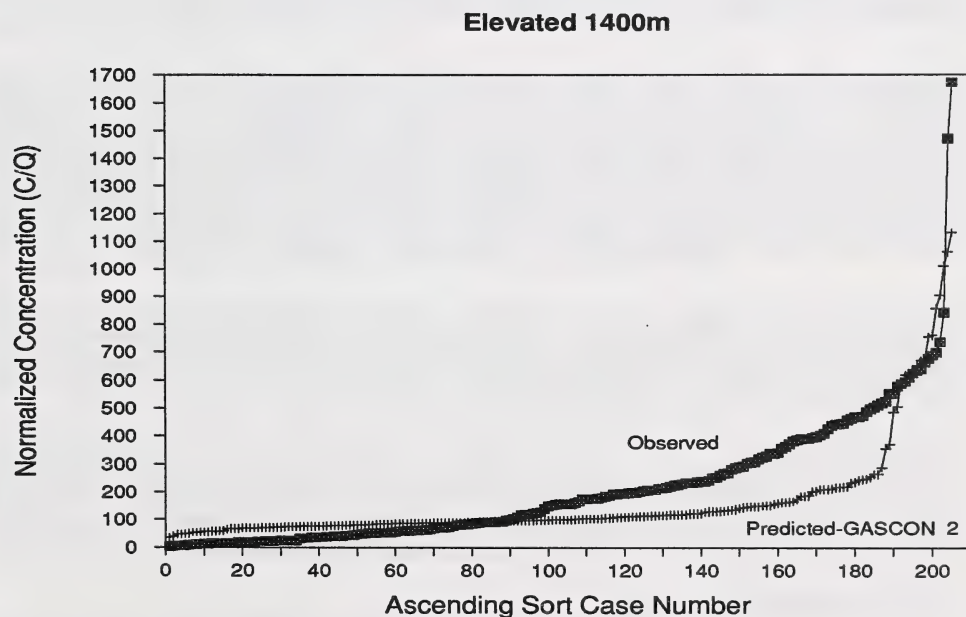
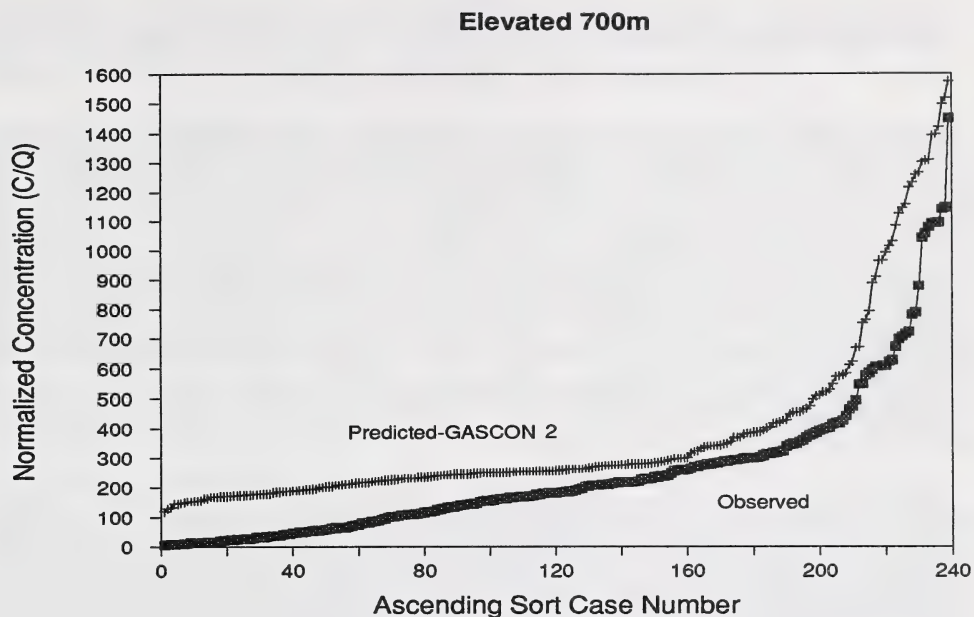


Figure 4.8

Unpaired GASCON2 Model Predictions and Observed Concentrations for Elevated Releases Normalized by Tracer Release Rate and Sorted Independently by Normalized Concentration.

Table 4.3**Summary of Fractional Bias Statistics**

Case	Observed C/Q Range (ppt/g/min)	Number of Cases	Fractional Bias (Average)	Fractional Bias (Std.Dev.)
Ground--700 m	5000-11000	45	0.28	0.07
Ground--1400 m	700-4400	14	0.46	0.32
Elevated--700 m	400-1500	31	-0.34	-0.09
Elevated--1400 m	400-1700	33	0.23	-0.07

Models that predict accurately will have fractional biases near zero. The bias of the average indicates the model's ability to estimate the average of the concentration range under consideration, while the bias of the standard deviation represents the model's ability to predict the distribution of concentrations over that range. Negative fractional biases indicate overprediction and positive fractional biases represent underprediction. As a guideline, the EPA may require models for regulatory use to have fractional biases below 0.67, which is equivalent to a difference in average predicted and observed values of a factor of two.

As seen in Table 4.3, all cases easily meet the EPA guideline of having a fractional bias below 0.67. Therefore, the average of the worst case scenarios could be predicted within a factor of two, although not paired in time and space. Additionally, the relatively small fractional biases of the standard deviations indicate that the predictions of these cases will be distributed similarly to the actual observed concentrations. The highest fractional bias of the average occurs for ground releases at the 1400 m arc. This value of 0.46 is equivalent to an average underprediction of 60% in the region of worst case conditions.

This analysis is limited by two important factors. First, the model input parameters available from the original paired data set may not cover the entire range of meteorological conditions that resulted in the observed dispersion values. Consequently, the model may have not been given the chance to predict the peak observed values.

Secondly, GASCON2 predicts three minute average concentrations, while the tracer traverse data provides essentially instantaneous maximum concentrations. Instantaneous values will always be higher than time averaged values due to plume meander. Methods of correcting results from one time average to another are discussed in Section 4.4.4.

4.4.3 Case Study - Test 15

To address some of the limitations of the model evaluation described in the previous section, a subset of the data was chosen for a case study. Test 15 was judged to be the most representative of worst case conditions, based on the occurrence of many of the highest C/Q values of all test periods. The ground release was typified by wind speeds at 4 m elevation of under 2 m/s, wind speeds at 10 m elevation of less than 3 m/s, and strong thermal stability indicated by vertical temperature gradients ranging from +0.22 to +0.35 °C/m. The elevated release period experienced wind speeds at 4 m elevation averaging below 3 m/s, wind speeds

at 10 m elevation ranging from 3 to 4 m/s, and a somewhat less stable vertical temperature gradient ranging from +0.13 to +0.22 °C/m. Temperature throughout the ground and elevated release periods stayed fairly constant at -22 to -24 °C.

In the top graph of Figure 4.9, the model predictions originally generated in the paired data analysis for the Test 15 ground release and the observed tracer concentrations have been normalized by the release rate and sorted independently by ascending values of observed normalized concentration (C/Q). The model consistently underpredicts the observed concentrations. Additionally, this graph illustrates the dramatic difference in model predictions for stable and neutral conditions. The flat part of the predicted concentration curve represents model outputs for which the meteorological preprocessor determined conditions to be neutral. The section of the curve that tracks the observed values are outputs for conditions determined to be stable. Low wind speeds and large positive temperature gradients indicated extreme stability throughout this period. Consequently, the meteorological preprocessor did not correctly predict stability for all cases during this period.

The original meteorological inputs matched to traverse data may not have included all the conditions resulting in worst case dispersion. To account for this, all three minute averages of meteorological inputs for the entire ground and elevated release periods during the test were used to predict three minute average concentrations, without regard to the existence of observed tracer data. This ensured that the model had access to data on all meteorological conditions that resulted in the observed concentrations. Due to uncertainties in the heat flux values for three minute averaging times, the heat flux was set to a constant -10 W/m^2 , representing a moderately stable atmosphere. All other meteorological parameters were used as in other field data runs.

The predicted and observed values of C/Q for the complete meteorological data run were sorted independently in ascending order and plotted on a scale normalized by the total number of cases. This provides an even distribution of both predicted and observed values for comparison purposes. The results of the ground release at the 700 m arc are presented in the lower graph of Figure 4.9. When given access to the entire range of meteorological data, the model follows the trend of the observed data very closely, and ultimately overpredicts the peak observed concentration by approximately 40%.

Similar results for the elevated release period later in Test 15 are shown in Figures 4.10 and 4.11. When only the predictions resulting from the meteorological inputs originally paired with the traverse data are used, the model apparently underpredicts the observed data by as much as a factor of four. When the full range of meteorological inputs are used, portions of the predicted curve match the observed curve quite closely. However, a section of the predicted curve tends to dramatically overpredict the observed concentrations. Since most of the elevated release period was conducted during a period of decreasing stability, it is likely that these higher predicted C/Q values result from stable conditions earlier in this period during which tracer data was not collected.

4.4.4 Comparison of Plume Dispersion Coefficients

Concentrations of substances dispersed in a plume are a function of the wind speed along the plume transport direction and the plume dispersion in the horizontal and vertical planes. Consequently, any model is limited by its ability to predict plume dispersion coefficients. Only horizontal plume dispersion coefficients (σ_y) can be determined from the tracer data;

they have been calculated using the moment method fit described in Volume 1 of the FMP report series. Comparison of the predicted and observed values of σ_y should provide a more fundamental indication of GASCON2's ability to predict plume dispersion.

Paired observed and predicted σ_y values were sorted by ascending observed σ_y concentrations. The results for ground releases are shown in Figure 4.12 and for elevated releases in Figure 4.13. (For clarity, the highest values of σ_y 's have been excluded to provide a distinguishable scale.) Smaller σ_y 's indicate lower dispersion and would result in higher normalized concentrations. The larger predicted values of σ_y which are relatively constant result from conditions classified as neutral by the meteorological preprocessor. The more variable, smaller σ_y values were produced under conditions classified as stable. There is no apparent correlation between the paired predicted and observed values of σ_y . As discussed previously, this lack of correlation may be due to a combination of mismatched meteorological data and misinterpretation of the data by the meteorological preprocessor.

To overcome the limitations of the paired analysis of dispersion coefficients, the predicted σ_y values were resorted in ascending order independently of the observed σ_y values. The results for ground releases are shown in Figure 4.14 and for elevated releases in Figure 4.15. The region of smallest σ_y values represents worst case conditions of low dispersion resulting in high normalized concentrations. In general, the observed σ_y values in this region are a factor of 1.5 to 2 smaller than the predicted values. By itself, the difference in predicted and observed σ_y values would result in the model underpredicting observed concentrations by this same ratio.

The effects of the difference in averaging times between the model predictions and the field data have not been included in this analysis. Crosswind plume dispersion increases with increased averaging time due to plume meander. Section 8.7 of Volume 1 of the FMP report series describes a power law formula which may be used to account for this increased dispersion:

$$\frac{\sigma_{y2}}{\sigma_{y1}} = \left(\frac{t_2}{t_1} \right)^p \quad (4.10)$$

where t_1 and t_2 represent the averaging periods associated with horizontal plume dispersion coefficients σ_{y1} and σ_{y2} . High frequency wind data collected by sonic anemometers during the Field Measurement Program were used to calculate crosswind (σ_y and σ_θ) for various time periods. The exponent p in the above power law relationship was estimated from these results for various stability classes and time average ranges. For stable conditions and time corrections in the range of 1 second to three minutes, the exponent p was estimated to be 0.2.

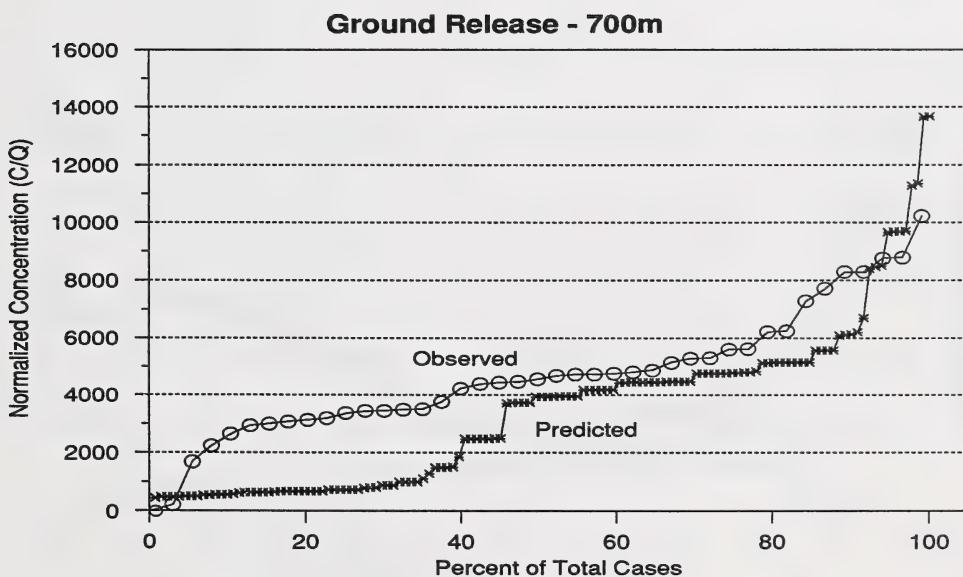
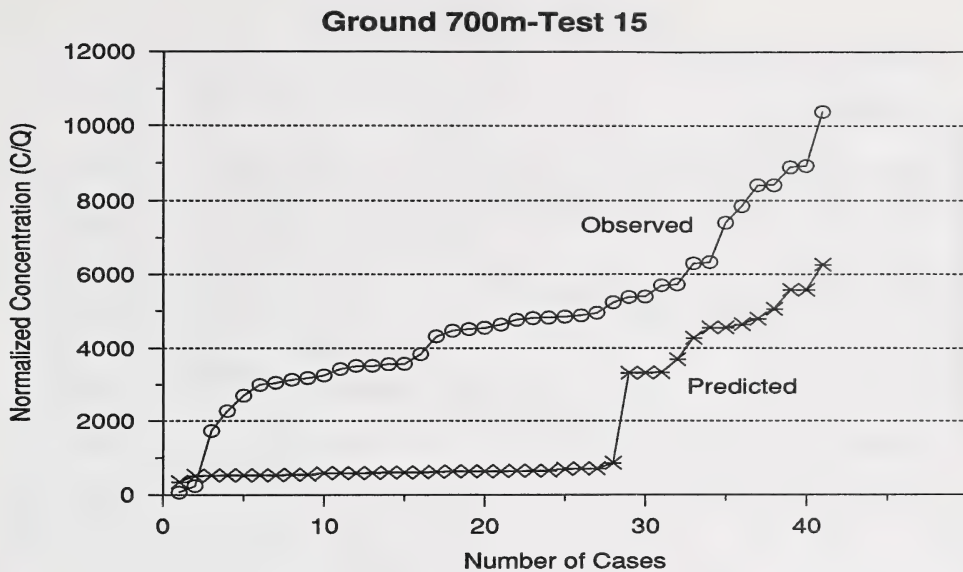


Figure 4.9

Unpaired GASCON2 Model Predictions and Observed Concentrations for Test 15 Ground Releases at the 700 m Arc Normalized by Tracer Release Rate and Sorted Independently by Normalized Concentration. The Top Figure is an Unpaired Analysis However, it Uses Only Predictions Generated Originally in the Paired Analysis; The Bottom Figure Uses Predictions From 3 Minute Meteorological Data for the Entire Ground Release Period.

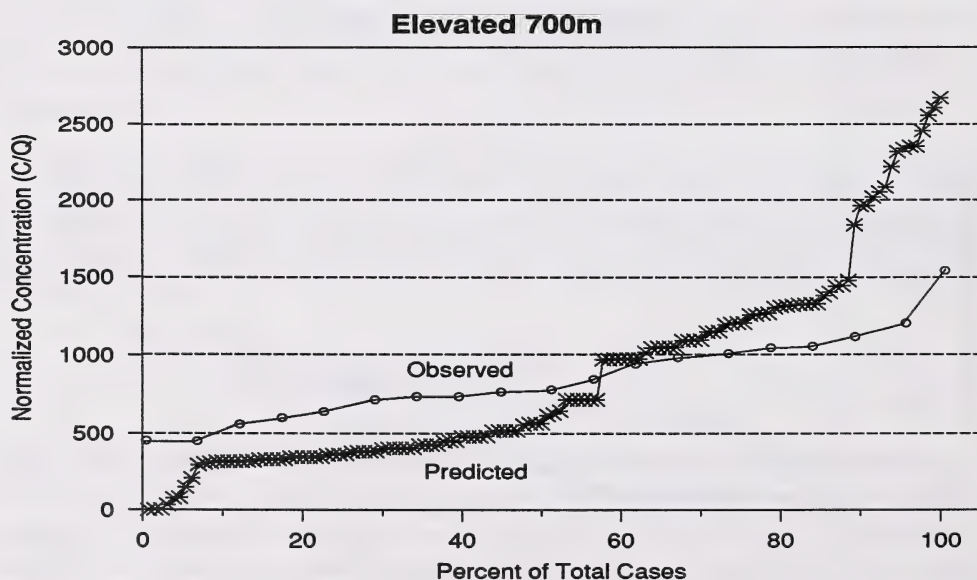
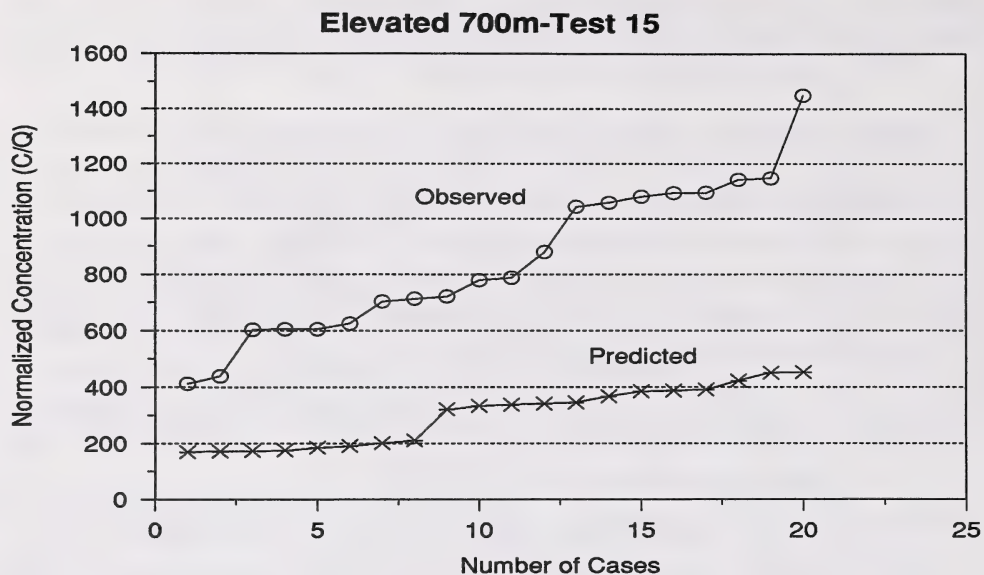


Figure 4.10

Unpaired GASCON2 Model Predictions and Observed Concentrations for Test 15 Elevated Releases at the 700 m Arc Normalized by Tracer Release Rate and Sorted Independently by Normalized Concentration. The Top Figure is an Unpaired Analysis However, it Uses Only Predictions Generated Originally in the Paired Analysis; The Bottom Figure Uses Predictions From 3 Minute Meteorological Data for the Entire Elevated Release Period.

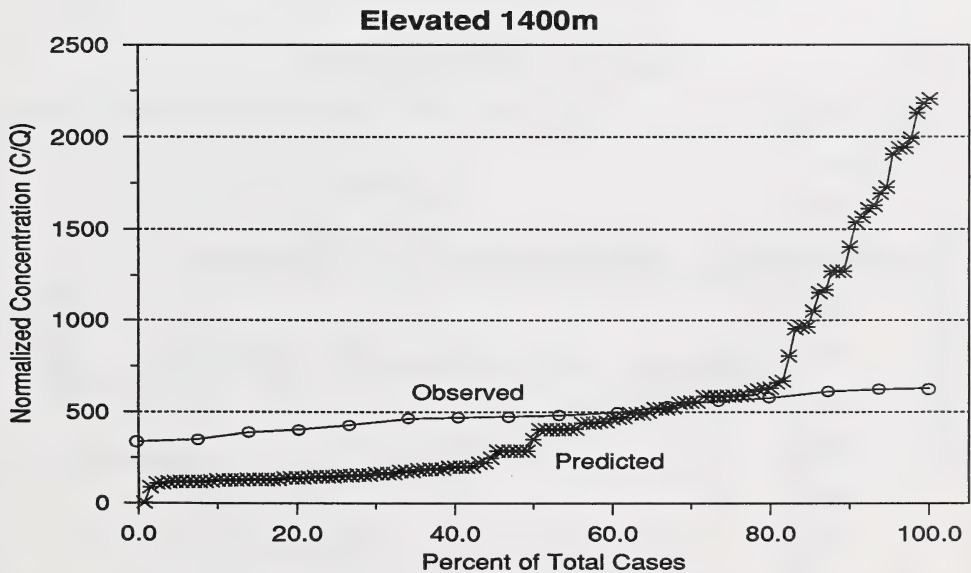
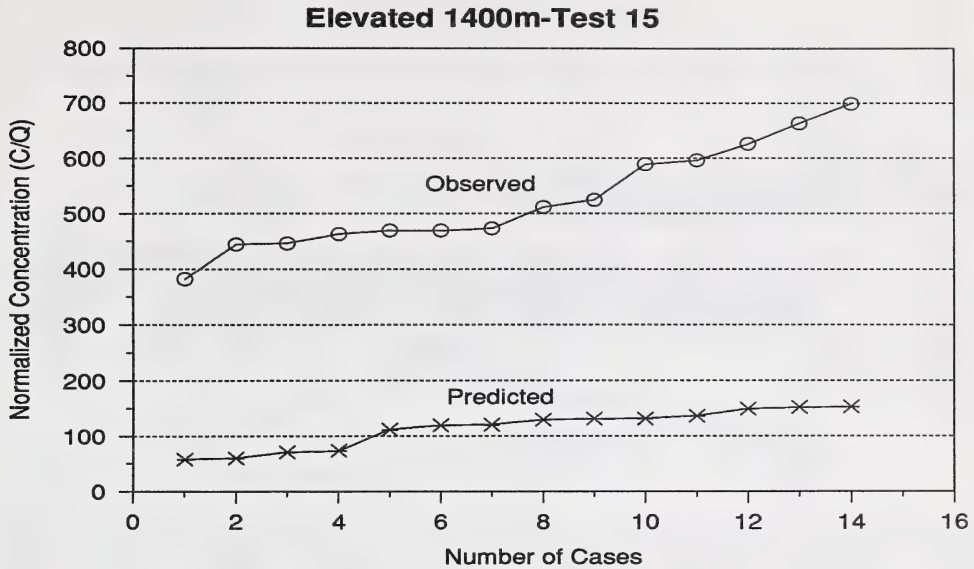


Figure 4.11

Unpaired GASCON2 Model Predictions and Observed Concentrations for Test 15 Elevated Releases at the 1400 m Arc Normalized by Tracer Release Rate and Sorted Independently by Normalized Concentration. The Top Figure is an Unpaired Analysis However, it Uses Only Predictions Generated Originally in the Paired Analysis; The Bottom Figure Uses Predictions From 3 Minute Meteorological Data for the Entire Elevated Release Period.

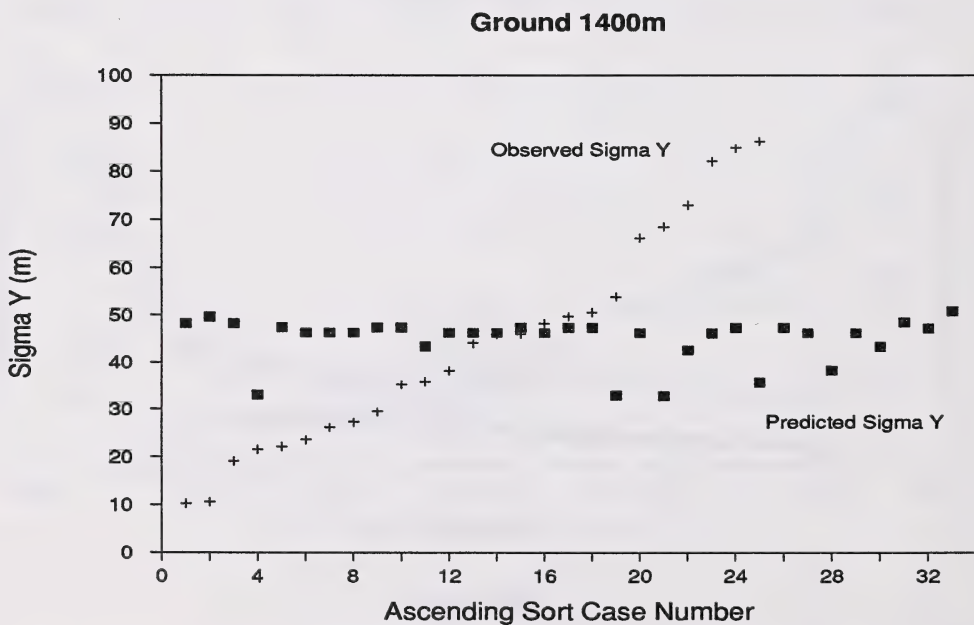
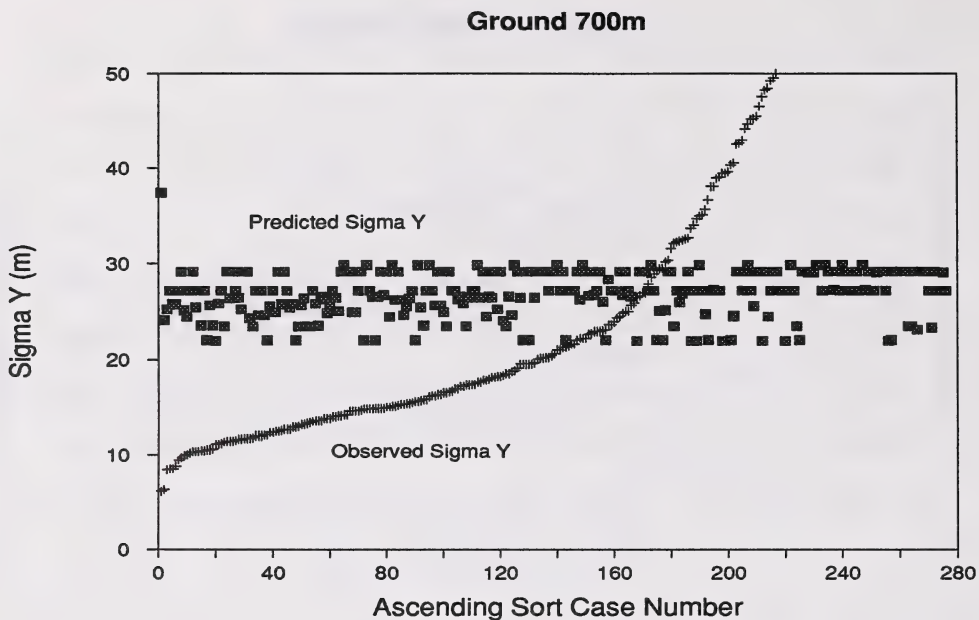


Figure 4.12

Paired GASCON2 Model Predictions and Observed Values of Horizontal Plume Dispersion Coefficients (σ_y) for Ground Releases at the 700 m and 1400 m Arc, Sorted by Observed σ_y .

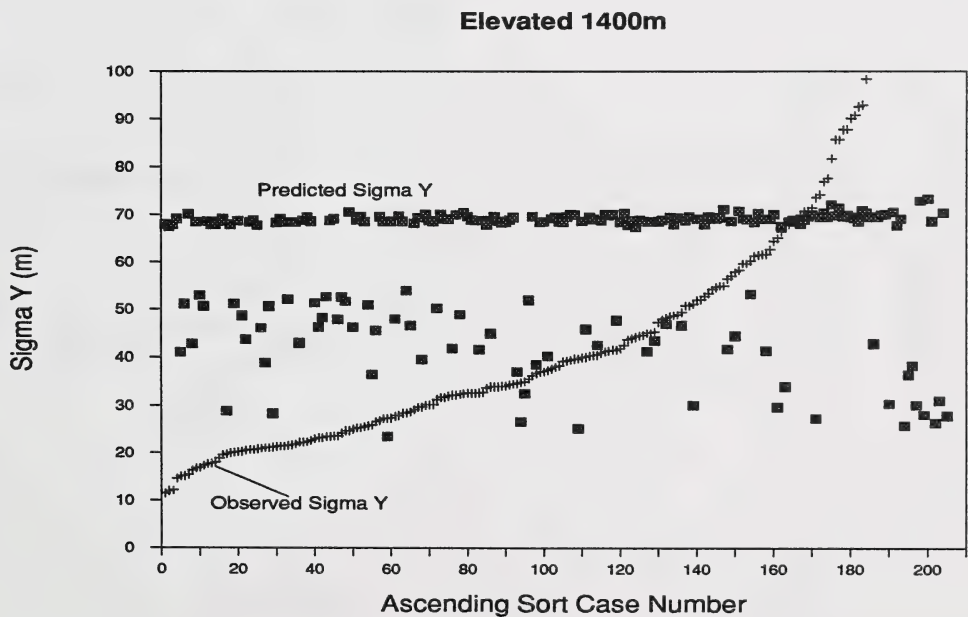
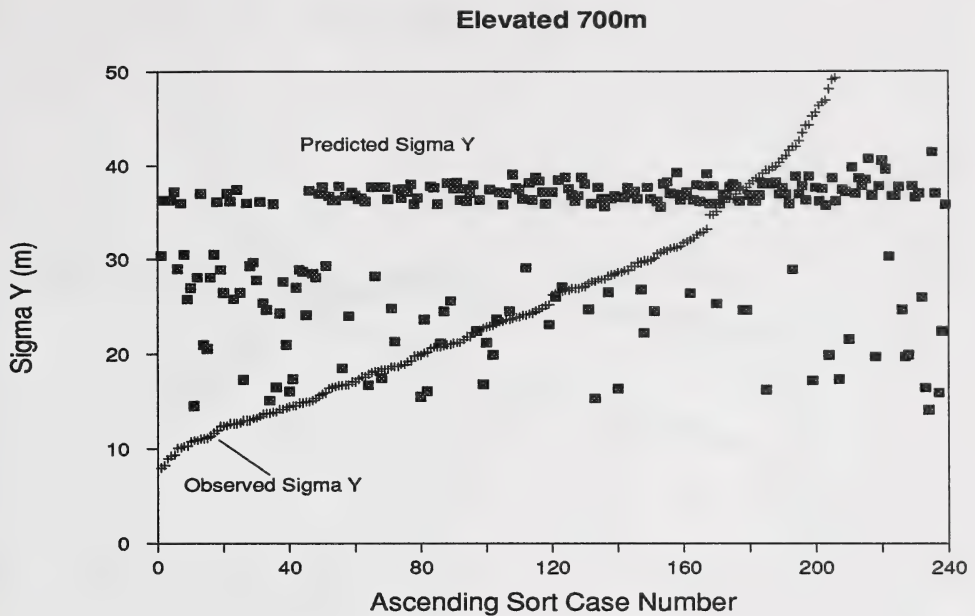


Figure 4.13

Paired GASCON2 Model Predictions and Observed Values of Horizontal Plume Dispersion Coefficients (σ_y) for Elevated Releases at the 700 m and 1400 m Arc, Sorted by Observed σ_y .

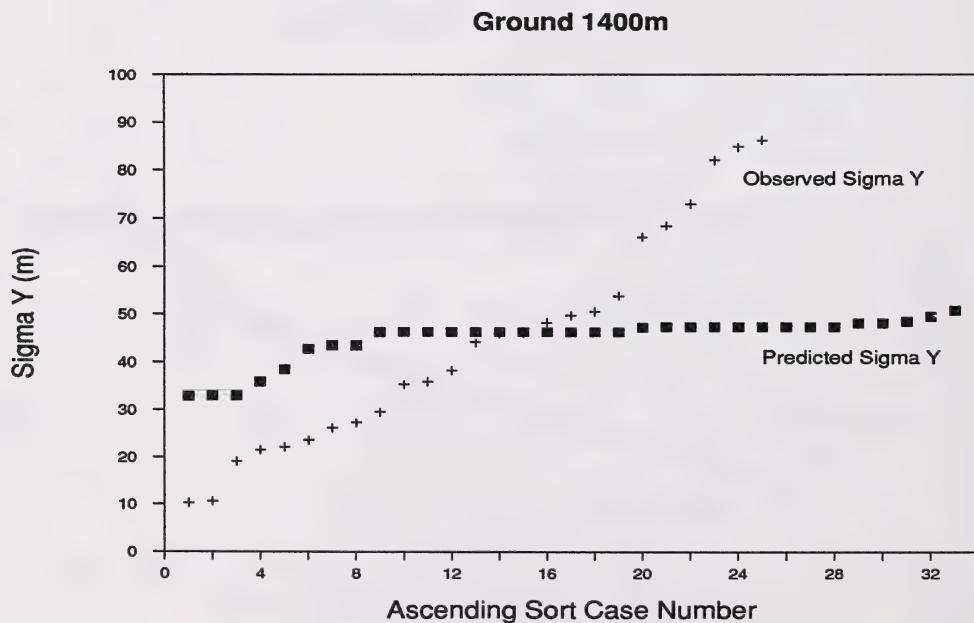
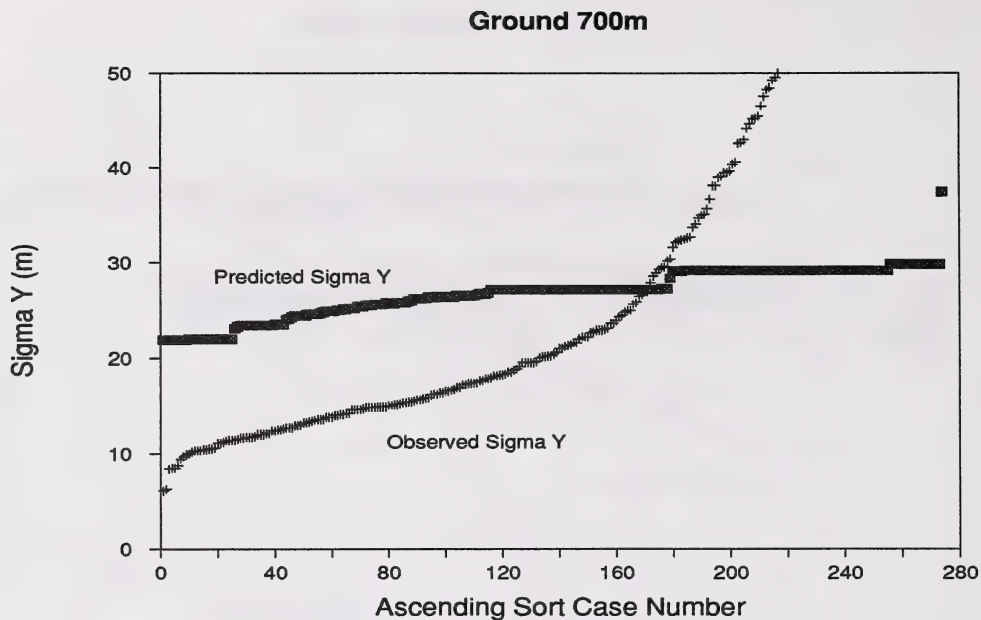


Figure 4.14

Unpaired GASCON2 Model Predictions and Observed Values of Horizontal Plume Dispersion Coefficients (σ_y) Independently Sorted by σ_y for Ground Releases at the 700 m and 1400 m Arc.

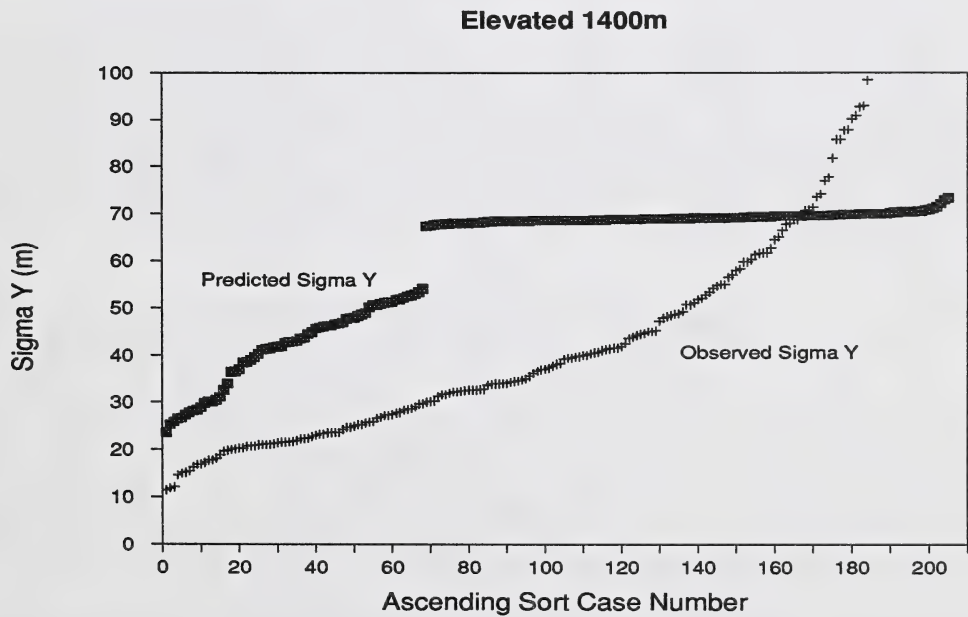
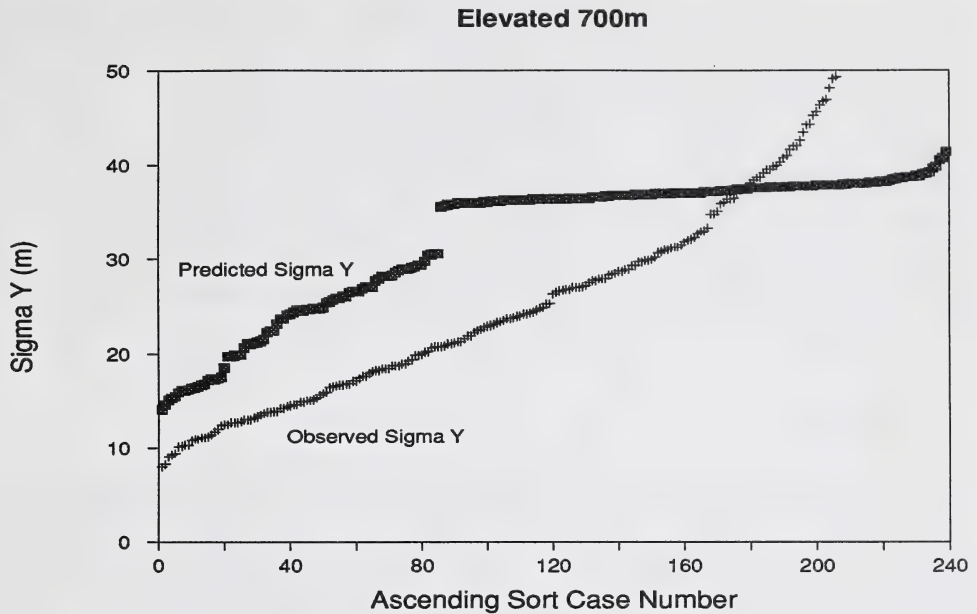


Figure 4.15

Unpaired GASCON2 Model Predictions and Observed Values of Horizontal Plume Dispersion Coefficients (σ_y) Independently Sorted by σ_y for Elevated Releases at the 700 m and 1400 m Arc.

The time average represented by an analyser vehicle traverse is somewhat uncertain. Although the concentration measurements were essentially instantaneous, there was a finite transport time of the analyser through the plume. Additionally, this transport time was affected by both the speed and direction of the plume meander with respect to the analyser vehicle motion. Typical travel times through the tracer plumes ranged from approximately 30 to 60 seconds. A range of correction factors can be assigned based on an averaging time of this order. For traverses equivalent to a 60 second average, the three minute average σ_y would be 1.25 times larger than the σ_y calculated from the traverse. For a 30 second time average, the three minute average σ_y would be 1.43 times larger. If these corrections were applied to the σ_y values predicted by GASCON2, the difference in predicted and observed σ_y values would then range from approximately 10 to 60%.

4.5 Summary

Tracer dispersion data and meteorological data collected during the Field Measurement Program have been used to investigate the performance of the dispersion module of GASCON2. Model predictions were generated by using meteorological inputs averaged over the transport time from the meteorological tower to the sampling arcs. However, uncertainties were introduced in matching these inputs to traverse data since the tracer release location was often not close to the meteorological tower.

Comparisons were made of the predicted and observed data sets using analyses which were both paired and unpaired in time and space. In general, the results of the paired analyses did not show a good correlation between the predicted and observed values. The correlation coefficient (r) was 0.17 for ground release cases and 0.28 for elevated cases. The ground release predictions were within a factor of two of the observed concentrations for 23% of the cases while 40% were within a factor of two for the elevated cases. When the paired data set was sorted by concentration normalized by the release rate (C/Q), the model predictions showed an increasing tendency of underprediction in the higher normalized concentration ranges.

The results of the unpaired analyses were much better. Normalized concentrations (C/Q) were sorted independently for the predicted and observed data sets. The fractional bias was calculated for the worst case concentration regimes for ground and elevated release concentrations at the 700 m and 1400 m arcs. All four of these cases easily met the U.S. Environmental Protection Agency guideline of having a fractional bias less than 0.67. This requirement is equivalent to the average of the predicted values being within a factor of two of the average of the observed values. The largest difference in the averages of the worst case predicted and observed concentrations was 60% for the ground release at the 1400 m arc. Additionally, small fractional biases of the standard deviations for these cases indicated that the model also predicted the distribution in these ranges accurately.

There is some uncertainty in the matching of meteorological data inputs to the model to the tracer dispersion data, as well as in the meteorological preprocessor classifications of stability conditions. For these reasons, the unpaired analysis probably provides the most realistic evaluation of GASCON2. Based on this analysis, the dispersion module of GASCON2 can predict the worst case concentrations that might occur during a toxic release with reasonable accuracy (within a factor of two). It is not clear at this point whether or not GASCON2 can predict plume concentrations at the correct place and time with this same level of accuracy.

Appendix A

PAIRED MODEL EVALUATION ON 1987 GASCON VERSION

A PAIRED MODEL EVALUATION FOR 1987 GASCON VERSION

A.1 Model Evaluation Summary

GASCON was originally developed in June 1987 and was first evaluated after the Field Measurement Program in early 1990. Since then many changes have been incorporated into the new model, GASCON2, taking into account the field work and current research. It was thought that old model evaluation runs (on 1987 GASCON) might be useful to compare to the new (1990 GASCON2) runs and as such the old runs have been included in this appendix. It should be noted that only paired analyses appear in this 1987 GASCON evaluation appendix whereas the 1990 GASCON2 evaluation, in the main body of this report, has both paired and unpaired analyses. This appendix appears as it was originally written with minor editorial changes.

The evaluation runs utilized varying amounts of model and field data to ensure that performance sensitivity to differing inputs was evaluated. The three major runs that were undertaken are depicted in Figure A.1 as options and they are as follows:

Option 1 • Model Generated U^* , Monin-Obukhov length (L) and Temperature Gradient

Surface heat flux, ambient temperature and pressure, surface roughness, wind speed and mixing height (when available) were used as the field inputs into GASCON.

Option 2 • Field U^* , Monin-Obukhov length (L) and Temperature Gradient

Field U^* , Monin-Obukhov length and temperature gradient were used as inputs in GASCON in addition to the Option 1 field parameters.

Option 3 • Field σ_v and σ_w

This model run incorporated field values for σ_v and σ_w as additional field input data.

In addition to the three main options the final analysis included:

- An analysis of the impact of removing the integral plume rise component of GASCON and using the passive dispersion (Figure A.2).
- A breakdown of each option into drainage and non-drainage winds (Figure A.2).
- A further breakdown by stability, elevation and wind speed (Figure A.2).
- A review of the way in which the traverse data was binned. This was to provide a better ensemble average considering that the model predicted an ensemble mean. One limitation of this method was that only one parameter could be binned at a time.

OPTIONS FOR MODEL 1 COMPARISON (GASCON)

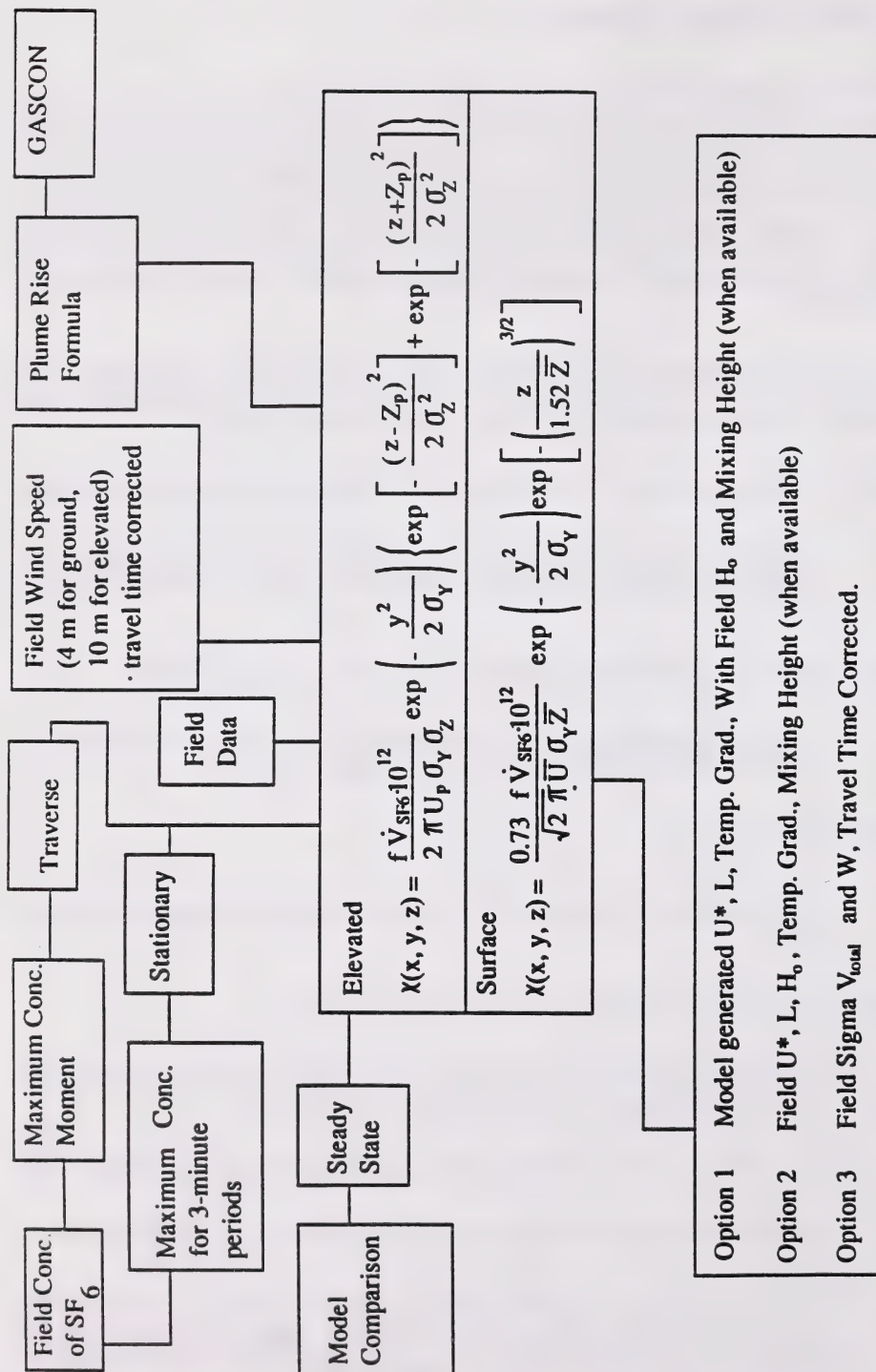


Figure A.1

GASCON Model Comparison Options

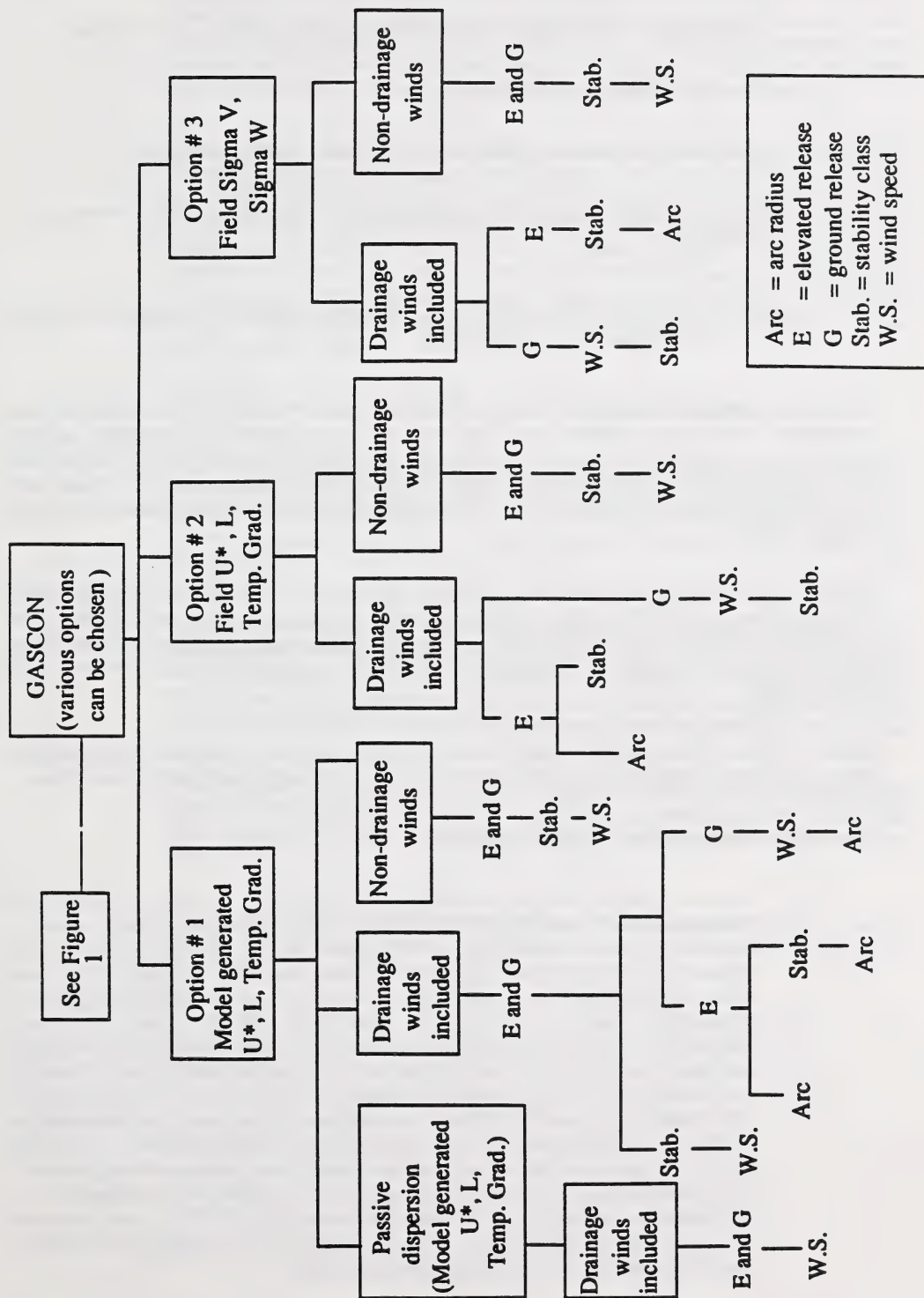


Figure A.2
GASCON Factor of 2 Analysis

- A review of both the mean and median values of predicted over observed.
- A summary of the model performance using the factor of 2 and 3 values.
- Detailed statistics for the three options.
- Graphical presentation of the results which are explained further.
- A case study designed to evaluate model performance under "worst case" conditions.

A.2 Option 1 -Model Generated U^* , Monin-Obukhov Length (L) and Temperature Gradient

This option utilized GASCON as it was originally designed. The only field meteorological parameters used were surface heat flux, ambient temperature and pressure, surface roughness, wind speed and mixing height (when available). The field mixing height data was obtained from a combination of acoustic sound and tether sonde data. This parameter is only utilized when the stability class is unstable otherwise the model generated its own mixing height.

In addition, field surface heat flux was generated from data at the 10 meter sonic anemometer. If the data was missing, Equation 3.5 (from the main body of this report) was applied. The ambient temperature and pressure were averaged over the duration of the test while the surface roughness used was averaged monthly. Steady mass and SF_6 flow rates were also input directly.

Figure A.3 shows six separate graphs. The set of three graphs on the left are for all possible cases. The set of three graphs on the right are for just low wind speed, stable conditions.

For all possible cases (on the left of Figure A.3):

The top graph (Graph 1) shows the log base 2 ratio for predicted concentration/observed maximum concentration (Moment method) versus a cumulative percent. The data has been sorted by the log base 2 ratio, as this represents a factor of two deviation for predicted over observed. Over and under predictions are indicated by positive and negative values of $\log_2 (P/O)$ respectively, with a perfect correlation indicated by zero. Predicted concentration in the ratio refers to GASCON three-minute time averaged concentration while the observed refers to the corresponding field observed maximum concentration using the Moment method. The tails of the S-shaped curve refer to the traverses where the model poorly predicted the concentration relative to the field observed value (either over or underpredicted). If the data points had been on a horizontal line there would have been perfect agreement. The curve intersects the zero line at approximately 50% which indicates very little skewness towards over or underprediction by GASCON. Any points on the curve which fall between -1 and 1 on the y axis indicate the model is predicting within a factor of two for that traverse.

The second from top graph (Graph 2) depicts the medians of the log base 2 concentration ratio versus wind speed. This graph shows that at low wind speeds (less than 3 m/s), the model overpredicts concentration while at higher wind speeds, GASCON tends to slightly underpredict. Since these transects never sampled the true maximum concentration in the plume, GASCON would very likely overpredict the apparent observed maximums for these cases.

The final graph (Graph 3) is a histogram presenting the percentage of cases where the model predicts concentration within a factor of two, factor of three and greater than a factor of three. Negative log base 2 values show underprediction by GASCON and positive values indicate overprediction by GASCON. GASCON predicts the observed concentration within a factor of two for 42% of the cases as can be seen from this graph. It should be noted that these plots include both elevated and ground release traverses. Drainage wind cases ($U_4 > U_{10}$) and unusual wind profiles between the four and ten meter sonics ($U_{10} > 3U_4$) were deleted from the data set.

For just the low wind speed, stable condition cases (on the right of Figure A.3):

Again the second set of graphs are similar to the first set except they are plotted for cases where GASCON indicated stable conditions and wind speeds less than 3 m/s. The top cumulative curve (Graph 1) crosses the zero line at about 45 percent indicating the data is slightly skewed toward overprediction by GASCON.

Graph 2 shows the plot of the median values of the log base 2 concentration ratio versus wind speeds (less than 3 m/s). For wind speeds less than 2.5 m/s and stable conditions, GASCON generally overpredicts. For wind speeds of 0.5 m/s and 1.0 m/s, there is more uncertainty, and therefore performance at these low wind speeds may not be truly indicative of overall model performance.

The histogram (Graph 3) also shows the skewness towards overprediction with about 25% of the data overpredicted by a factor greater than three. GASCON predicted the field observed concentration within a factor of two for 41% of the cases.

As indicated previously, the overpredictions at low wind speeds must be viewed with caution. This region may be influenced by traverses parallel to the plume center line.

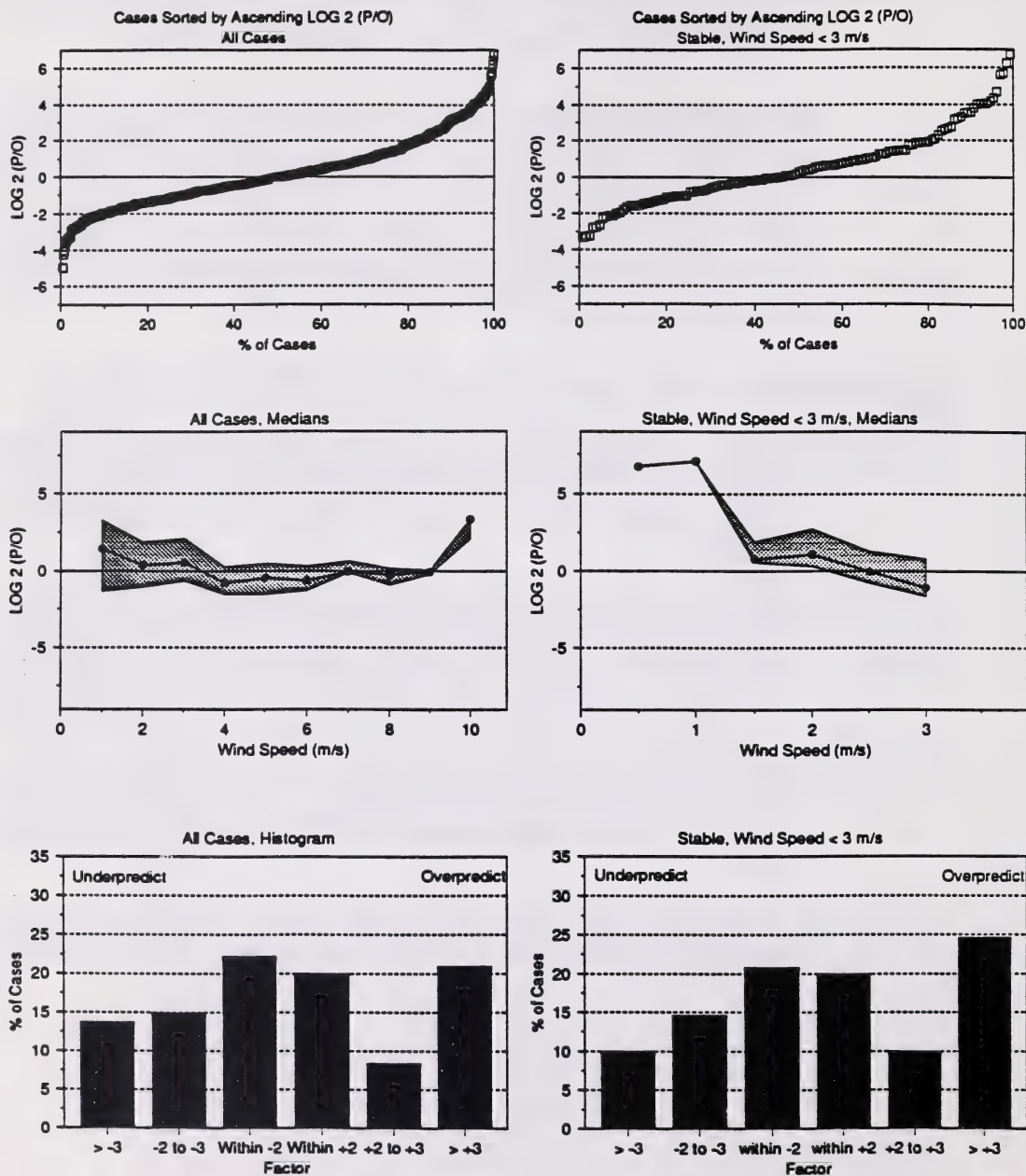


Figure A.3

Paired GASCON Model Comparisons for Elevated and Ground Releases for Option 1

A.3 Option 2 -Field U^* , Monin-Obukhov Length (L) and Temperature Gradient

Additional field meteorological data was used for this set of evaluation runs. The surface velocity scale (U^*) and the Monin-Obukhov length were travel time averaged from three-minute 10 m level data. Travel time averaging involves averaging individual 3 minute data blocks over the time required for the plume to travel from the source to the analyser. The temperature gradient used was the travel time averaged temperature difference between the 25 meter and 2 meter tower levels. Other meteorological inputs (surface heat flux, temperature, etc.) were identical to their use in Section A.2. The drainage winds ($U_4 > U_{10}$) and irregular profile winds ($U_{10} > 3U_4$) were deleted from the final data set along with any traverses in which the field U^* , L or temperature gradient data was missing.

For all possible cases (on the left of Figure A.4):

Figure A.4 again shows the same three graphs on the left in the same format as Section A.2. Graph 1 shows there is very little skewness in the data set. The second graph again shows GASCON generally overpredicting at wind speeds less than 3 m/s. Also GASCON predicted the field observed moment concentrations within a factor of two for 51.1% of the cases (see Graph 3). This is a 10% increase over Section A.2.

For just the low wind speed, stable condition cases (on the right of Figure A.4):

The graphs on the right are for low wind speed, stable condition traverses. The data set is skewed as shown in Graph 1. The curve crosses the zero line between 35% and 40% suggesting GASCON overpredicts more than it underpredicts at low wind speed, stable conditions. The overprediction at low wind speeds is further indicated by Graph 2. This is supported by Graph 3 which shows that for approximately 35% of the cases, GASCON overpredicts by greater than a factor of three. Predicted concentrations within a factor of two were found for 40.3% of the paired cases. This is about the same as in Section A.2 for low wind speed, stable cases.

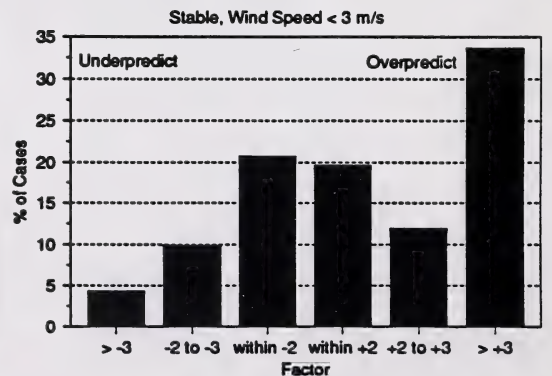
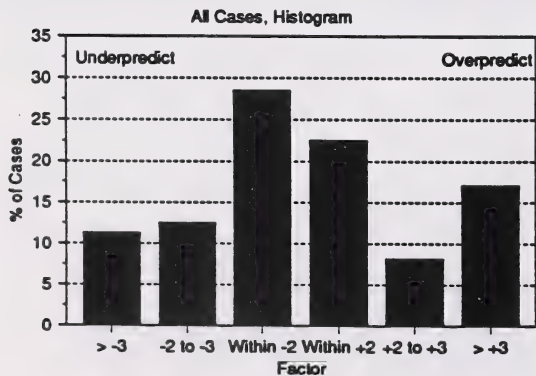
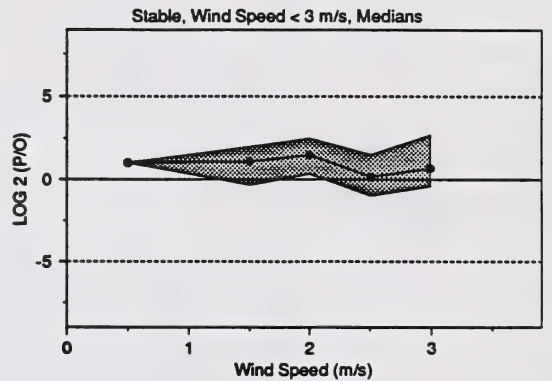
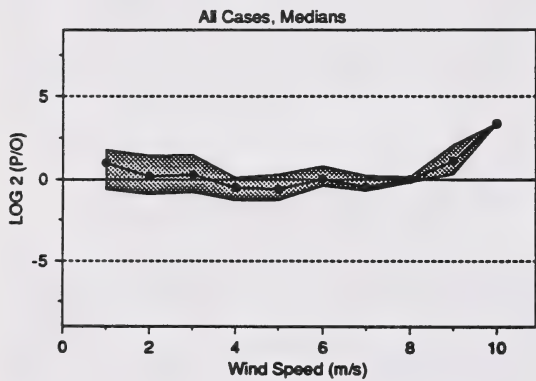
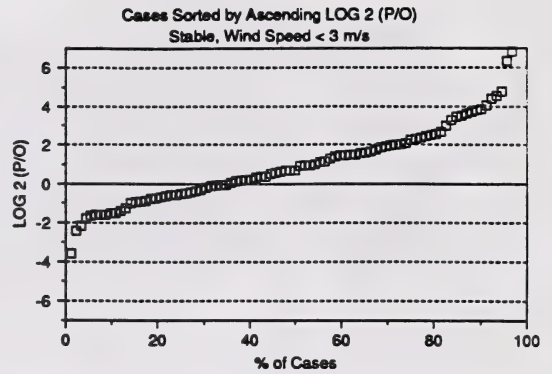
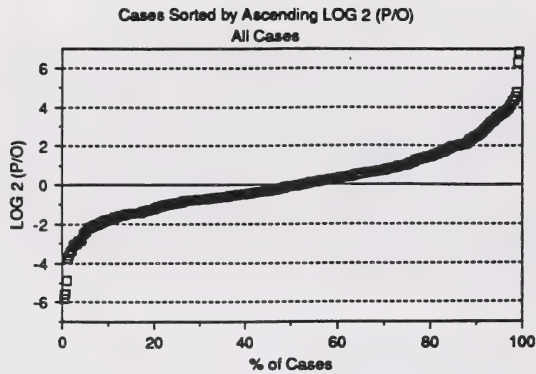


Figure A.4

Paired GASCON Model Comparisons for Elevated and Ground Releases for Option 2

A.4 Option 3 - Field Sigma V and Sigma W

Field travel time-averaged sigma V (σ_v) and sigma W (σ_w) from the 10 meter level were included as an additional input for this run. The other meteorological inputs such as ambient temperature and pressure were the same as in Section A.2. The model internally generated U^* , Monin-Obukhov length and temperature gradient as well. Drainage winds and irregular wind profile data were again deleted from the data set along with any traverses in which either the field σ_v or σ_w were missing.

For all possible cases (on the left of Figure A.5):

The format for the graphs again followed the format established in Section A.1. Graph 1 in Figure A.5 shows a slight skewness towards underprediction for the complete data set. Graph 2 seems to indicate that GASCON slightly underpredicts at low wind speeds which is opposite to the data seen in the other two runs. This is confirmed by Graph 3 where GASCON predicted 41.9% of the cases within a factor of two. This is comparable to the results seen in Section A.2 but less than the run utilizing field U^* , L , and temperature gradient data.

For just the low wind speed, stable condition cases (on the right of Figure A.5):

The second set of graphs (Figure A.5) shows data for the low wind speed, stable condition criteria. The S curve in Graph 1 crosses the zero line to the right of 50% indicating a skewness towards underprediction which is shown in Graph 2 and 3. There is a definite indication that when field wind sigmas are used in the model, GASCON underpredicts at low wind speed, stable conditions. The model only predicted 31.3% of the cases within a factor of two under these conditions. This is 10 - 20% less than either of the other two previous runs.

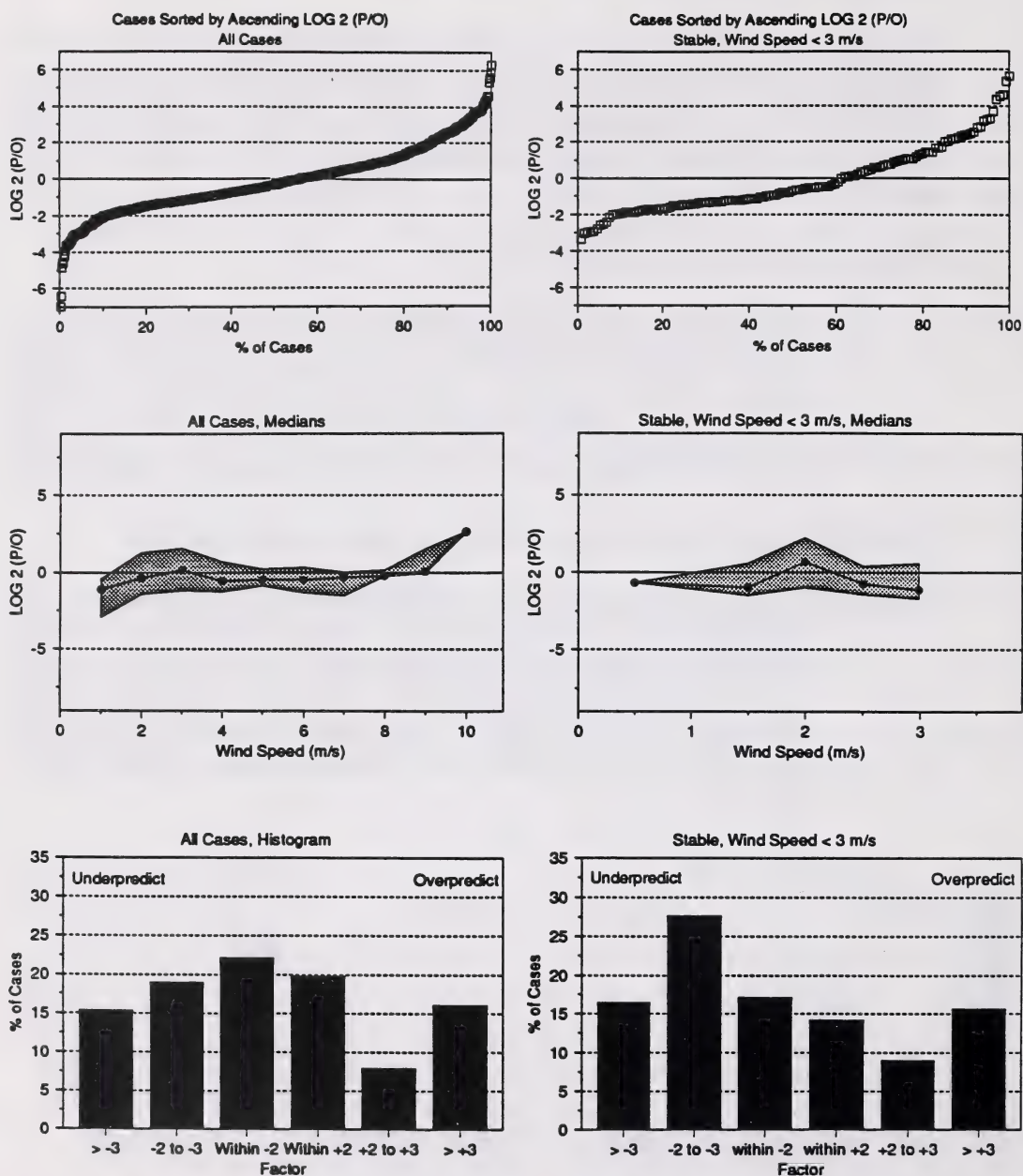


Figure A.5

Paired GASCON Model Comparisons for Elevated and Ground Releases in Option 3

A.5 Passive Dispersion Model Run

A modification was made to GASCON enabling a performance evaluation to be done on the passive dispersion module of the model. The plume rise was calculated normally rather than using the integral plume rise and then passive dispersion was applied over the full distance at the calculated height. The model used the appropriate virtual source distances.

All three options were run using this model version. It was found that the model performance, based on the factor of two evaluation technique, decreased using the passive module only. This applied to the low wind speed category as well as the full data set.

A.6 Factor of Two Analysis

One model performance parameter is the ability of the model being evaluated to predict paired field concentration values within a factor of two either high or low. Figure A.6, A.7 and A.8 show the factor of two analysis for the three model run options as well as the passive dispersion run. There is also a further breakdown of each run into stability classes, wind speeds, arc radius, source type and drainage wind classifications. Option 1 was more finely classified because it was the base case.

A number of comparisons both within an individual run and between runs can be made. In general, it appears that the Option 2 model run with field U^* , L , and temperature gradient inputs predicted the greatest percentage within a factor of two for both drainage and non-drainage wind cases. This inference also applies to the stable case where the Option 2 model run predicted 53.2% of the paired stable cases within a factor of two for the non-drainage wind classification.

Comparisons made within model runs themselves also show certain trends. Arc radius had some influence on the performance with elevated field concentration data obtained at 700 m arc showing better factor of two agreement than data obtained at the 1400 or 2100 m arcs. Wind speed also had some effect on performance. For both the drainage wind and non-drainage wind classifications, the performance of the model at wind speeds greater than 3.0 m/s was better than for wind speeds less than 3.0 m/s in both neutral and stable conditions. There did not appear to be any great difference in performance between ground and elevated release classifications or between stability classes (stable versus neutral).

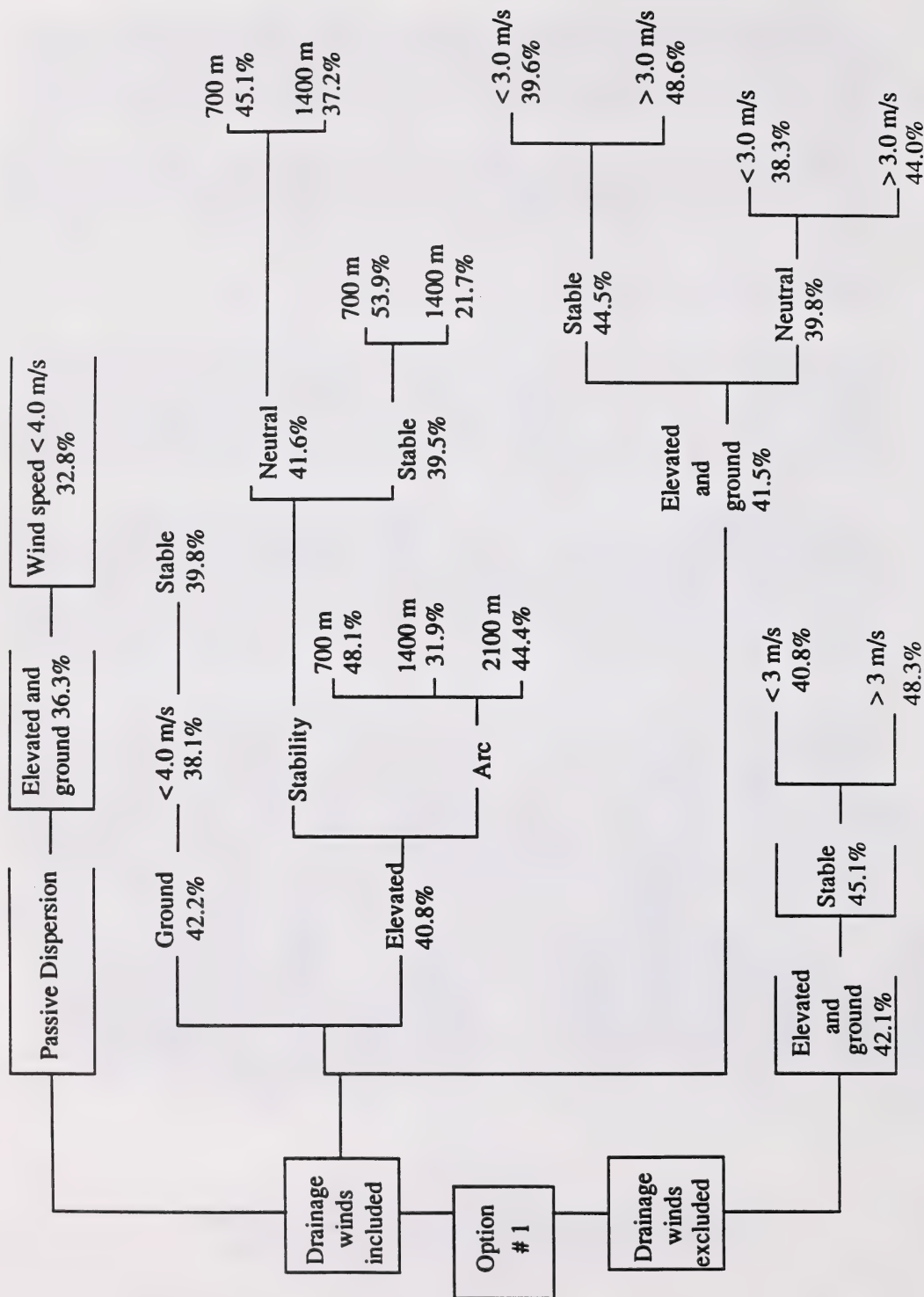


Figure A.6

Factor of 2 Analysis for Option 1

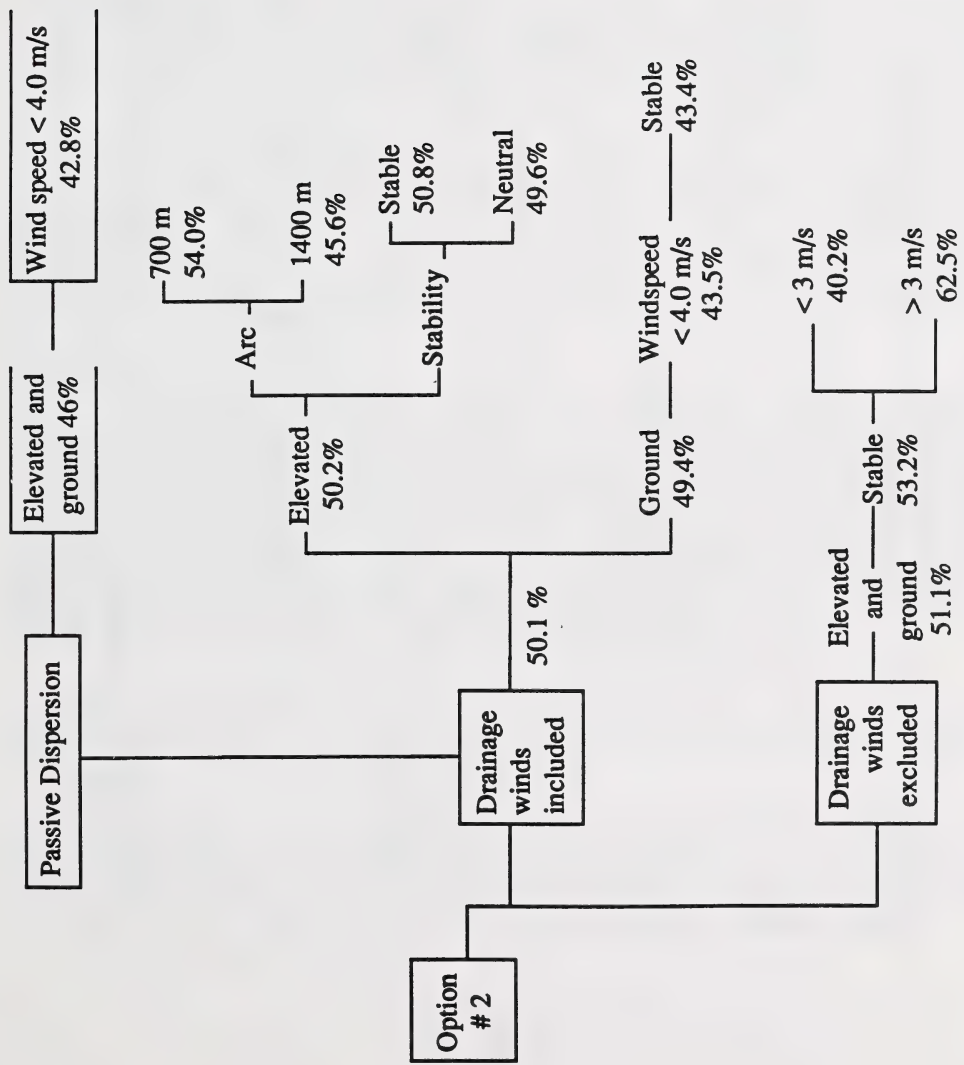


Figure A.7
Factor of 2 Analysis for Option 2

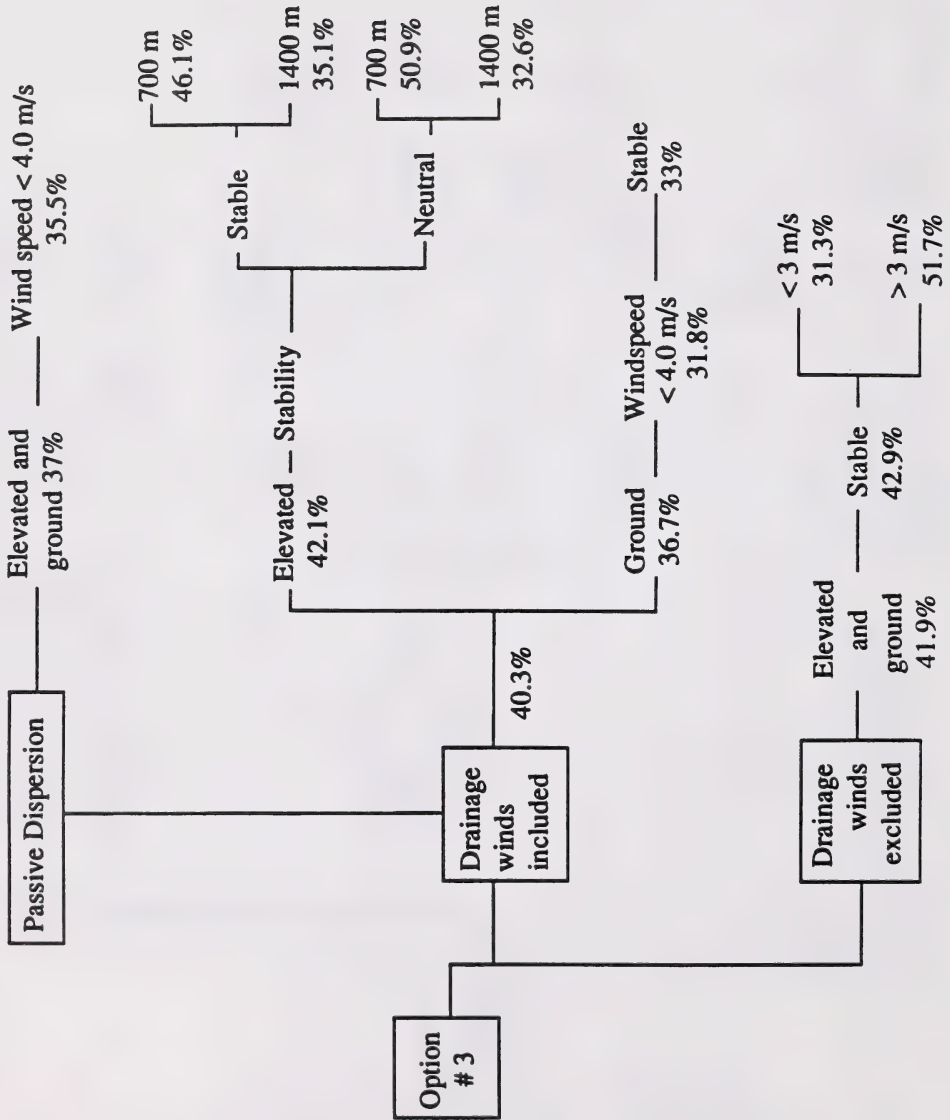


Figure A.8

A.7 Binned Versus Non-Binned Data Set

The Field Measurement Program concentration data presented in Figure A.9 is displayed in two formats: (1) binned and (2) non-binned by wind speed. One attempt to account for the fact that models predict ensemble means rather than instantaneous concentrations is to bin and take the mean within each bin. This can be done by binning parameters affecting dispersion. The parameter chosen was wind speed. This method has limitations as binning is by one parameter at a time.

In the binned format each point on the graph and its resulting average concentration are on an equal capacity basis. This means that each point represents the average of an equal number of cases. For the non-binned format, each point on the graph and its corresponding average represent all the cases contained in that bin. Each bin is of equal width but the number of cases contained in each bin will vary. Graphs a, c and e represent data in the non-binned format, while graphs b, d and f are in the binned format. Graph a is a concentration versus wind speed graph for all traverses from the Option 1 model run with drainage and irregular profile winds deleted. The graph shows that below 1 m/s, GASCON overpredicts the field observed concentrations but for wind speeds greater than 1 m/s, there is no real trend. Graph b is the same set of data but binned into equal capacity bins by wind speed. Each point on the graph represents the mean of approximately 25 traverses and therefore, each bin will not be the same width. This graph shows that from about 1.7 m/s to 2.6 m/s GASCON overpredicts, while greater than 3 m/s wind speed GASCON underpredicts.

The other four graphs all represent only traverses in which stable conditions prevailed. Graphs c and d use the same format as graphs a and b, while graphs e and f show the wind speed, non-binned and binned versus the log base 2 concentration ratio (as in Sections A.2 - A.4). Graph c again shows that for low wind speed (less than 2.5 m/s) stable conditions, GASCON overpredicts concentration. The same trend at low wind speeds is prevalent in graph d with GASCON overpredicting for conditions under 2.0 m/s, while for wind speeds higher than 2.0 m/s GASCON underpredicts. It should be noted however that for wind speeds lower than 1 m/s and stable conditions, there are only 2 traverses and therefore, conclusions at these low wind speeds must be made with caution. Graphs e and f show exactly the same trends that c and d did except in a logarithmic ratio format.

The conclusions to be drawn for this work is that for both the binned and non-binned methods, GASCON generally overpredicts at low wind speeds and underpredicts at higher wind speeds for both stable conditions as well as the entire data set.

The data presented in Figure A.10 shows heat flux data presented in the two formats (1) non-binned and (2) binned. Graphs a, c and e represent the binned format. The six graphs show a general trend for GASCON to underpredict at heat flux values less than -10 W/m^2 . For values of heat flux greater than -10 W/m^2 , the trend becomes much less clear.

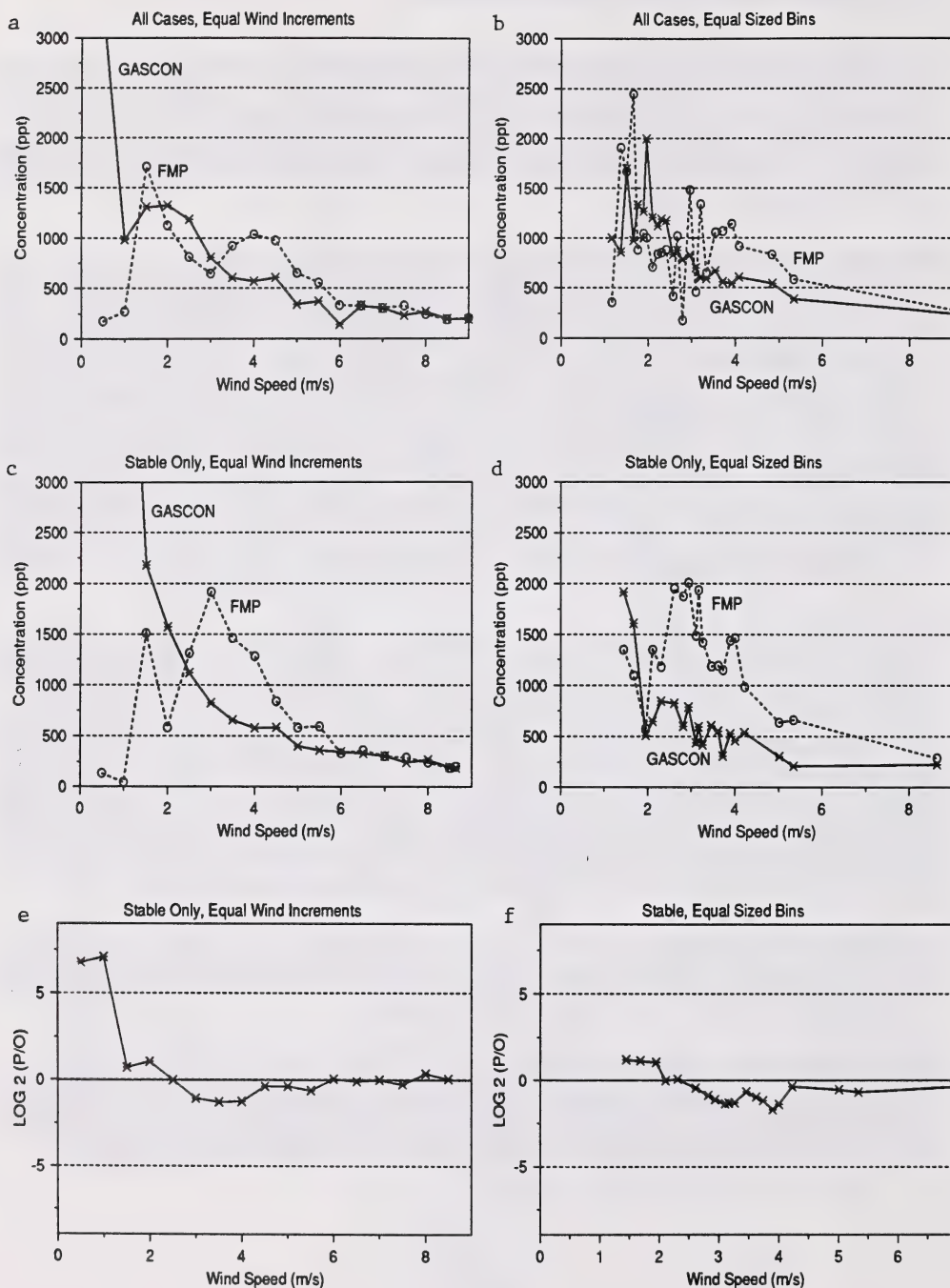


Figure A.9

Option 1 Model Comparison Using Binned versus Non-Binned Methods for Wind Speeds.

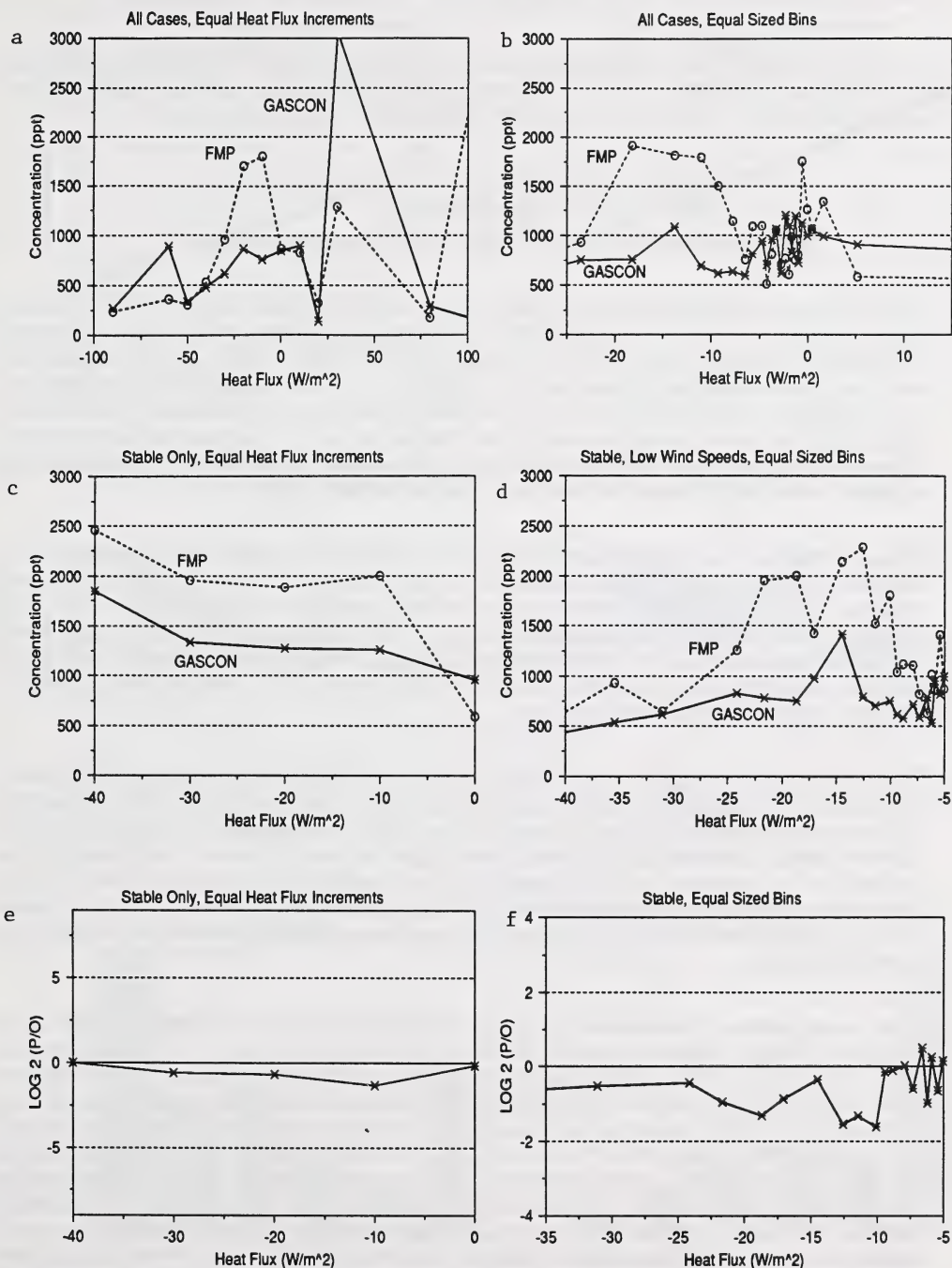


Figure A.10

Option 1 Model Comparison Using Binned versus Non-Binned Methods for Heat Flux.

A.8 Case Study: Low Wind Speed / Low Turbulence Occurrences

The technical committee identified conditions of minimal mixing in the tracer data set during low wind speed, low turbulence cases accompanied by low level inversion conditions as an area of importance. The following criteria were used to identify these cases:

- A) Wind speed at 16 m ≤ 2.0 m/s (low wind speeds)
- B) 16 m $\sigma_w \leq 0.1$ m/s (low turbulence)
- C) Maximum wind speed below 25 m (Drainage winds).

To investigate model performance during these conditions, predicted and observed values paired in time and space were compared. Ground and elevated releases were analysed separately. It should be noted that a few changes to GASCON (1987) were made and this case study is based on that updated version. In Figure A.11, the results of these comparisons are presented. In the top figures, $\log_2$ of the ratio of predicted and observed paired values ($\log_2(P/O)$) has been plotted against the distribution of cases. The same ratio is shown as a function of wind speed in the middle figures, followed by frequency distributions for the factor of two error between predicted and observed values.

The uppermost and lowermost figures indicate that GASCON tends to underpredict more frequently during ground release scenarios while tending to overpredict during elevated releases. The middle graphs show overprediction at very low wind speeds (0.5 - 1.5 m/s) for the ground releases with underpredictions at higher wind speeds. A similar trend exists for the elevated releases, but the crossover wind speed occurs at approximately 4 m/s. Note that the wind speed for the ground releases was measured at 4 m, and the wind speed for elevated releases was measured at 10 m.

Two important considerations may bias the results of this analysis. Because the predicted and observed values have been paired in time and space, the potential for errors caused by displacement of the meteorological measurements from the source and receptors increases as wind speeds decrease due to greater travel time between all points. Additionally, the probability for a traverse to travel through a plume parallel to the centreline and miss the true maximum concentration typically increases as wind speeds decrease and plume meander increases. For these reasons, paired analysis may be particularly misleading during low wind speed cases.

Also recommended for examination were cases of drainage winds and low wind speed, low turbulence cases for ground releases. These are presented in Figure A.12. Drainage winds were identified by wind speed maximums that occurred at levels below 25 m. Since the main wind field is decoupled from typical surface effects by the drainage flow, minimum vertical turbulence is expected and consequently may represent worst case conditions of low mixing. The drainage flows identified all fell within the Test 15 ground release period. All indications from this analysis point to a strong tendency for GASCON to underpredict during this period. However, the potential for mismatched model inputs and the difference between the three minute means predicted by the model and the instantaneous observed traverse data creates considerable uncertainty in this conclusion. Test 15 was also chosen for a particular case study based on the frequent occurrence of high normalized concentrations (C/Q). In that analysis, it was discovered that by performing an unpaired comparison of observed and predicted values, providing all three minute meteorological input periods to the model, and correcting for averaging time, that the model estimations during these suggested worst case conditions are within a factor of two or better of the observed values.

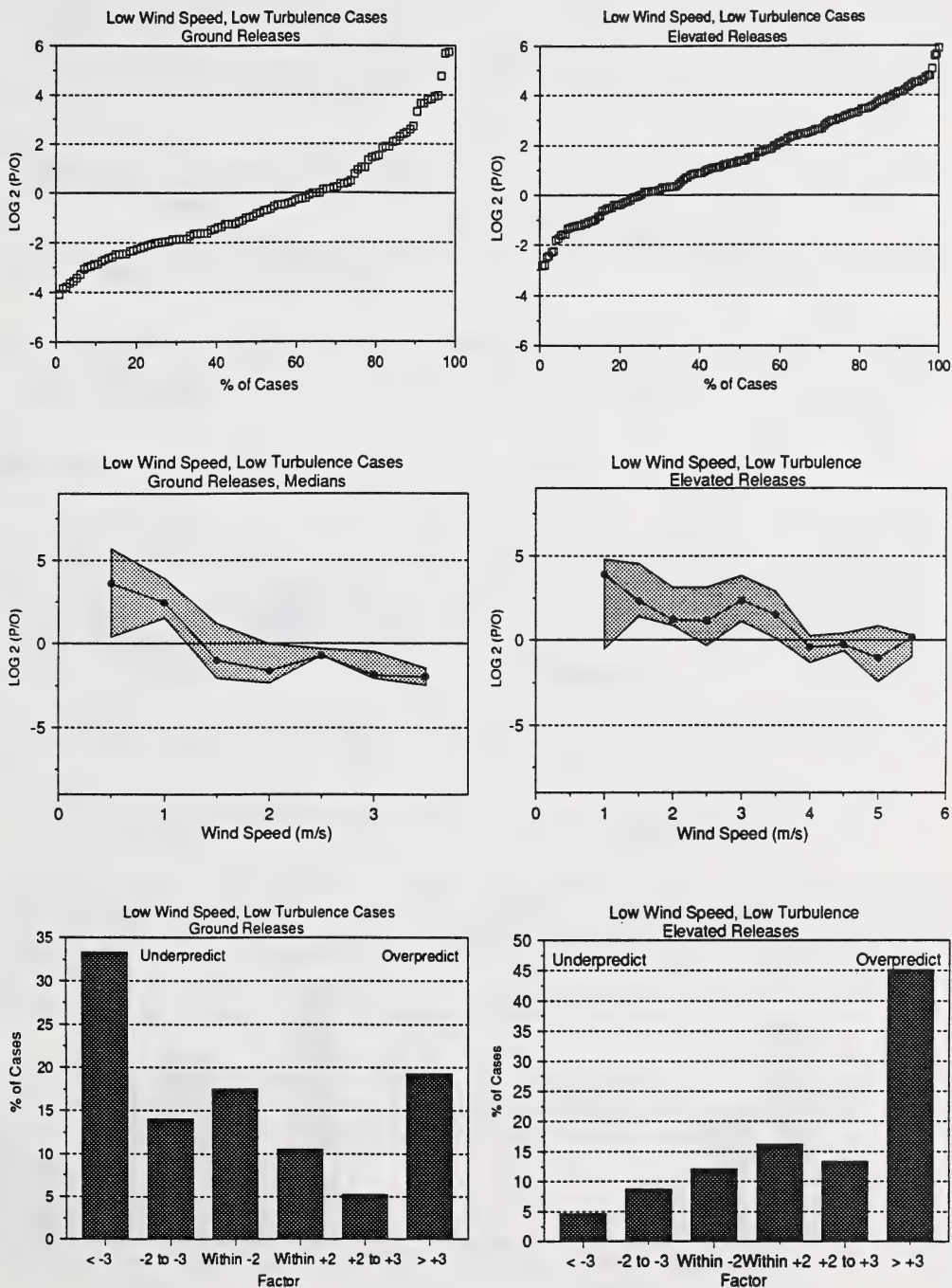


Figure A.11

Case Study of Periods of Light Winds and Low Turbulence Accompanied by Low-Level Turbulence Inversion Conditions for Elevated and Ground Releases.

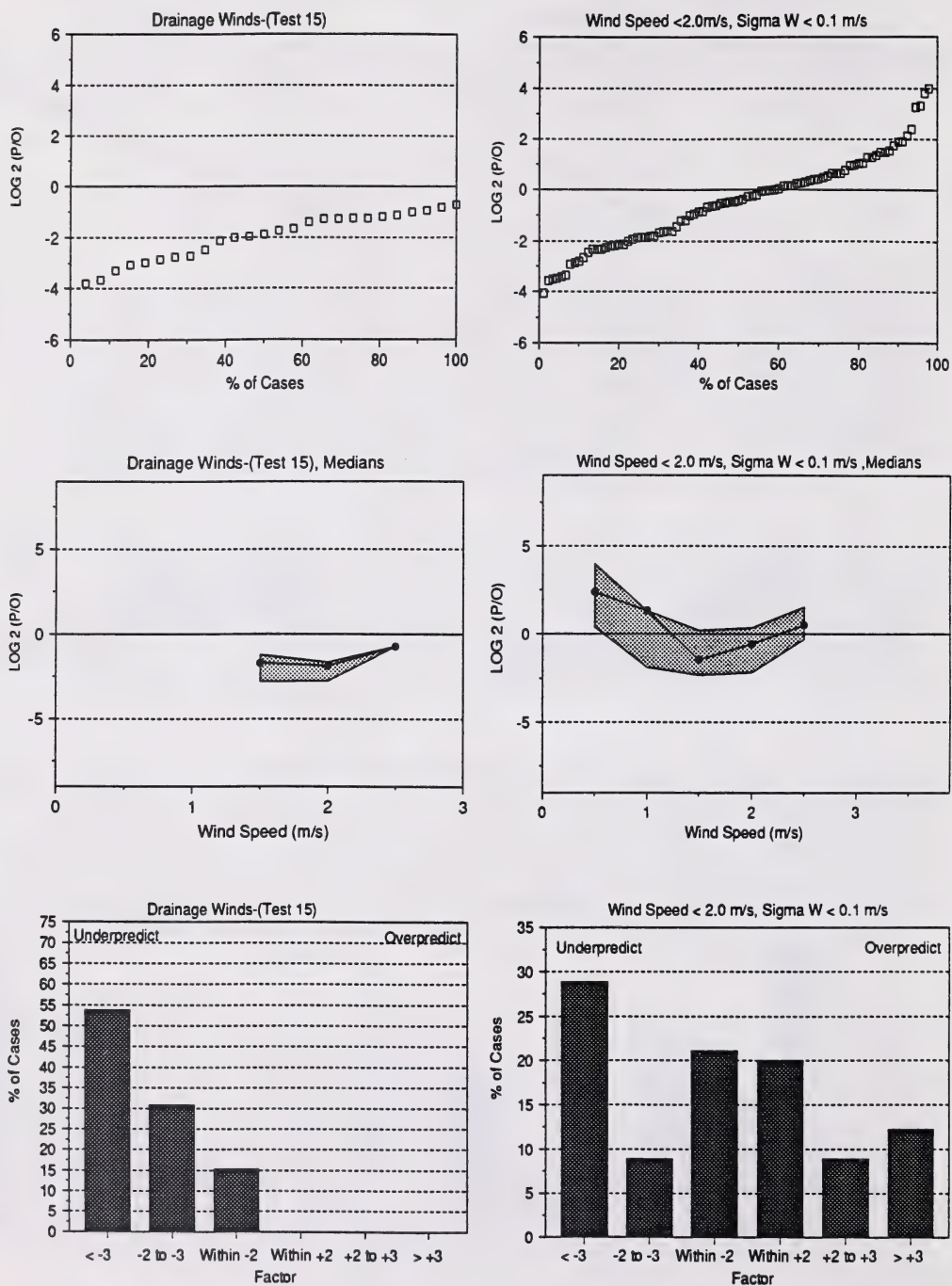


Figure A.12

Drainage Wind and Low Wind Speed, Low Turbulence Cases for Ground Releases.

The right hand side of Figure A.12 provides the same comparison for ground level cases with wind speeds below 2 m/s and σ_w less than 0.1 m/s. These cases do not exhibit a uniform tendency of either over or underprediction. This may be due to the lower range of wind speed where the mismatching of meteorological and traverse data and potential for parallel traverses becomes more significant.

A.9 Model Evaluation Statistics

Paired comparison statistics were generated for the three original option model runs (June 1987 version). See Table A.1.

The GASCON predicted three-minute concentration were compared to the paired essentially instantaneous Moment and Maximum Concentration method field concentration. The drainage and irregular profile wind cases were deleted for the Option 1-3 model runs.

Statistics

There are a number of statistics that can be generated. It is helpful to key in on certain factors such as the median *P* over median *O*. Models such as the gaussian are predicting ensemble means and one might assume that means should be compared, however, since the means were not always normally distributed the medians were considered to be the significant number to focus on. Again to avoid any concern with regard to this issue both medians and means appear in the table.

The factor of 2 analysis is another good statistic to look at. These values appear in the same tables and in graphical form for all of the paired data runs.

There are a number of generalizations that can be drawn from Table A.1:

Using the entire data set, Table A.1 shows that Options 1 and 3 were biased towards underprediction while Option 2 has an overprediction bias. Option 2 had the highest mean *P*/mean *O* ratio while Option 3 had the lowest. However, Options 1 and 2 were comparable when median *P*/median *O* ratios were examined while Option 3 again was lower. A further note to consider is that the values for the mean and medians are higher for the Moment method than the Maximum method generated field concentrations.

The conclusions to be drawn from these statistics are that the field U^* , L , and temperature gradient model run (Option 2) generally predicted the highest concentrations, was the most biased run and was the most accurate in terms of factor of 2 analysis.

Table A.1

Detailed GASCON Statistics - All Cases

	MEAN $\bar{P}$ $\bar{O}$	MEDIAN $\bar{P}$ $\bar{O}$	MEAN $\bar{O}$	MEAN $\bar{P}$	MEAN $\bar{P}$ $\bar{O}$	MEDIAN $\bar{O}$	MEDIAN $\bar{P}$ $\bar{O}$	$\frac{\text{MEDIAN } P}{\text{MEDIAN } O}$	R (P vs. O)	RMAE	HANNA's M	SLOPE	INTERCEPT	AVG. BIAS	MRE	% WITHIN FACTOR OF 2	% WITHIN FACTOR OF 3
OPTION 1 Moment Maximum (Non-drainage)	3.445 2.467	0.979 0.823	1266.8 1504.5	1140.7 1140.7	0.901 0.758	880.0 1015.0	742.6 742.6	0.844 0.752	0.178 0.187	0.805 0.749	2.138 2.250	0.189 0.163	901.3 895.6	126.0 363.7	0.705 0.682	42.1 43.6	65.3 67.5
OPTION 2 Moment Maximum (Non-drainage)	10.908 5.619	0.944 0.810	1242.1 1449.1	1846.9 1846.9	1.487 1.275	923.0 1072.0	802.5 802.5	0.869 0.749	0.059 0.070	1.256 1.119	13.203 11.324	0.263 0.267	1520.6 1459.5	-604.7 -397.8	0.653 0.638	51.1 50.4	71.7 72.6
OPTION 3 Moment Maximum (Non-drainage)	2.397 1.725	0.781 0.671	1265.1 1502.1	1113.9 1113.9	0.881 0.742	881.5 1020.0	672.9 672.9	0.763 0.660	0.246 0.247	0.823 0.776	2.696 2.665	0.350 0.289	671.3 680.0	151.2 388.2	0.687 0.678	41.9 41.5	68.9 69.4

A.10 Conclusions

This appendix contains the paired evaluation results for GASCON (Alp *et al* 1987). Varying amounts of field data were incorporated into three distinct sets of model runs (Options 1 to 3). The performance sensitivity to these varying inputs as well as an evaluation of the model could then be undertaken.

- Of the three option runs generated, Option 2 (field U^* , L and temperature gradient) predicted the observed concentration within a factor of two for the greatest percentage of cases (51.1%).
- GASCON generally overpredicted for wind speeds less than 3 m/s and underpredicted for wind speeds greater than 3 m/s for Options 1 and 2. Option 3 showed a general trend towards underprediction for all wind speeds.
- The performance evaluation made strictly on the passive dispersion portion of the model showed a decrease in factor of two performance for all three option runs.
- When Option 1 data was binned by wind speed, the same trend of overpredicting at low wind speeds and underpredicting at high wind speeds was prevalent. Data binned by heat flux showed a trend for GASCON to underpredict for heat flux values less than -10 W/m^2 and no trend for heat flux values greater than -10 W/m^2 .
- The table of statistics indicated that the field U^* , L and temperature gradient run (Option 2) generally predicted the highest concentrations, was the most biased and the most accurate in terms of factor of two analysis.
- GASCON can predict the observed concentrations within a factor of two approximately 50% of the time when paired in time and space.

These conclusions can be compared to the more recent model evaluation conclusions. This has been done in a general fashion in the main body of the report.

Appendix B

MODEL FRAMEWORK FOR 1987 GASCON VERSION

B MODEL FRAMEWORK FOR 1987 GASCON VERSION

This appendix contains the model framework for a slightly updated version of the 1987 version of GASCON. This has been included so that the results in Appendix A have some basis.

The GASCON model has been subdivided into a series of inter-dependent modules which can be used to estimate ground level concentrations and potential exposure zones corresponding to a given release scenario. As shown in Figure B.1, these modules include the:

- Mass Emission Rate,
- Jet Expansion,
- Plume Rise,
- Transient Release, and
- Passive Dispersion Modules.

The Mass Emission Rate Module (Section B1.1) estimates the sour gas release rate from well blowouts and pipeline ruptures. The well blowout portion of the module is trivial since the release rate is assumed to be constant with time. In contrast, the release rate from a pipeline rupture is a highly transient process, typically lasting no more than a few minutes.

The Jet Expansion Module (Section B1.2) simulates the initial behavior of the gas after its release to the atmosphere. Four "regions" are addressed:

- The Stagnation Zone which considers conditions at the jet exit,
- The Pressure Equalization Zone which considers the expansion of gas from the sonic, underexpanded state to atmospheric pressure,
- The Entrainment Zone which considers entrainment of ambient air into the jet, and
- The Combustion Zone which considers the potential ignition of the escaping gases.

These four regions of gas behavior are modelled as series processes.

The Plume Rise Module (Section B1.3) estimates the momentum and buoyancy rise of the jet after the jet expansion stage. Unlike usual plume rise estimates, this module can address non-vertical releases explicitly.

The Transient Release Module (Section B1.4) calculates an effective mass release rate for pipeline releases. The use of an effective mass release rate in the Passive Dispersion Module allows steady state dispersion formulations to be adopted for transient pipeline releases.

The Passive Dispersion Module (Section B1.5) estimates ground level plume concentrations as a function of distance from the release point. Unstable, neutral and stable atmospheres are considered. The turbulence in the atmosphere is allowed to vary continuously. Dispersion from elevated and surface releases are considered differently.

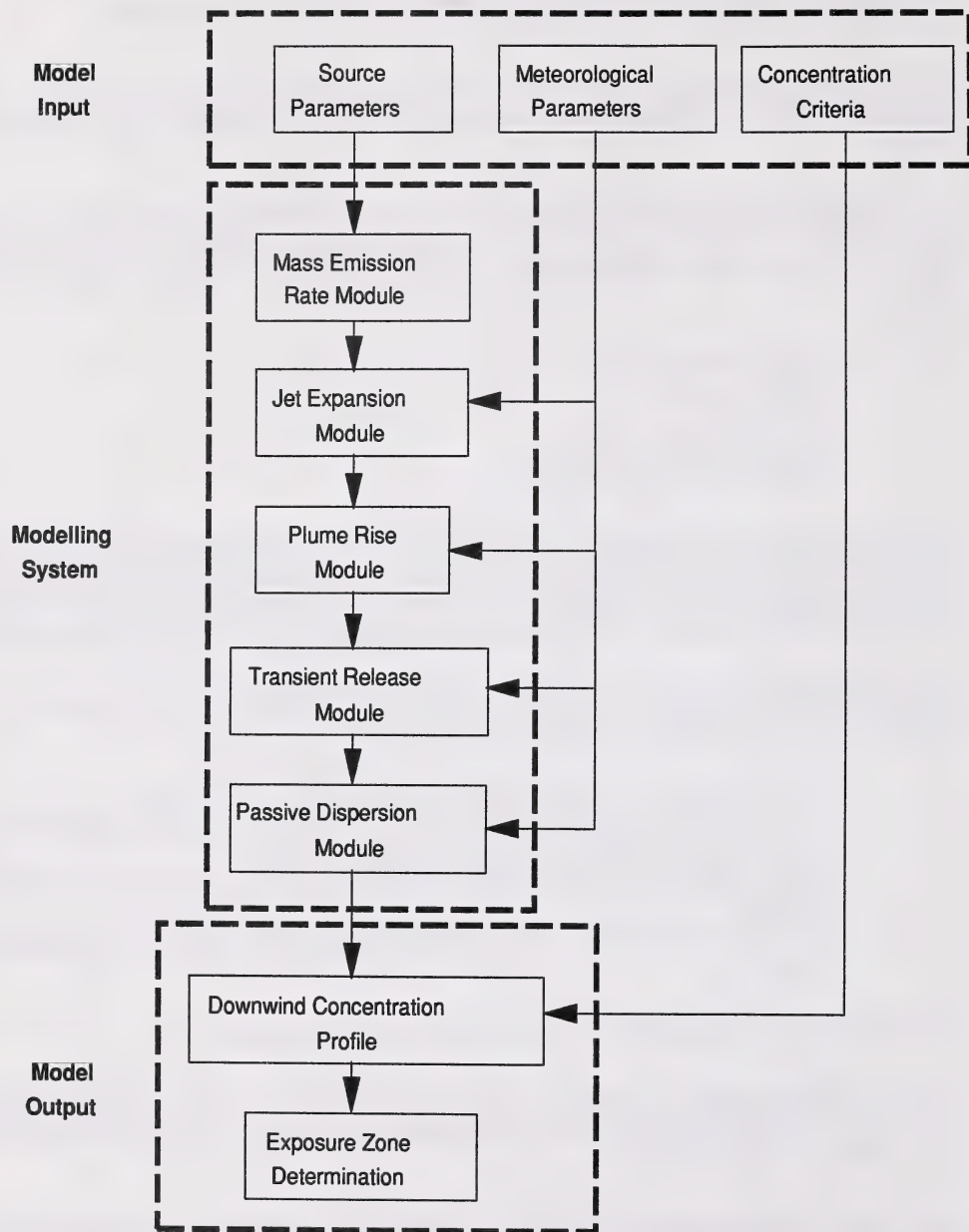


FIGURE B.1
Detailed GASCON Modelling Framework.

B1.1 Mass Emission Rate Module

The release rate of sour gas from potential uncontrolled discharges may be continuous (steady state) in the case of well releases or may be transient in the case of pipeline releases. Should an ESD valve fail at the well, then the release from a pipeline may have an initial transient component followed by a decay to a non-zero steady-state value.

Physical properties of the sour gas stream are required by the mass emission rate module (and by the jet expansion module). Specific properties of a gas stream "I" of known composition include the molecular weight (M_{wi}), heat of combustion (Q_{HI}), specific heat at constant pressure (C_{pi}) and the particular gas constant (R_i). Table B.1 indicates how these properties are calculated from the gas composition.

B1.1.1 Continuous Well Release

The deliverability of a well is usually expressed as a daily volume flow at a standard temperature and pressure of 15 °C and 101.3 kPa respectively. Of primary interest to the current dispersion modelling exercise, however, is the mass release rate of sour gas, denoted by $\dot{m}_E$:

$$\dot{m}_E = \frac{\bar{\rho} \dot{V}}{86,400} \quad (\text{B.1})$$

where: $\dot{V}$ = volume flow rate of sour gas (m^3/d)
 $\bar{\rho}$ = density of sour gas at standard conditions (kg/m^3)
 $\dot{m}_E$ = mass flow rate of gas (kg/s)

Since the volume flow rates are usually quoted for standard conditions (15 °C and 101.3 kPa), the density may be estimated from the ideal gas law:

$$\bar{\rho} = \frac{(101.3)(10^3)}{(288)R_E} \quad (\text{B.2})$$

where R_E = particular gas constant of the discharging gas ($\text{J}/(\text{kg} \text{ } ^\circ\text{C})$).

B1.1.2 Transient Pipeline Release

In contrast to well blowouts, the release of sour gas from a ruptured pipeline is a highly transient process, typically lasting no more than a few minutes. The nature of the release is dependent on the operating pressure of the pipeline, the size of the rupture and the length of pipeline isolated by emergency shutdown (ESD) valves. Since the volume of gas in the isolated section of ruptured pipeline is limited, the release is characterized by decreasing line pressure and decreasing mass flow rate.

Table B.1**Example of Gas Property Calculations.**

For a gas stream of known composition "I", the molecular weight M_{wi} of the combined gas stream can be calculated as the sum of the individual molecular weights weighted according to the individual mole fraction. As an example, for a typical sour gas stream:

Component	Mole Fraction	Molecular Weight	Product
C ₁	0.550	16.043	8.82
C ₂	0.005	30.070	0.15
C ₃	0.001	44.097	0.04
C ₄	0.001	58.123	0.06
H ₂ S	0.300	34.076	10.22
CO ₂	0.123	44.010	5.41
N ₂	0.020	28.013	0.56
Total:			25.27

The molecular weight of the gas stream is 25.27 kg/kmole. The heat of combustion (Q_{HI}) and the specific heat at constant pressure (C_{PI}) are calculated in a similar manner. Values for the individual molecular weights, heats of combustion and specific heats at constant pressure can be obtained from the SI Engineering Data Book (Gas Processors Suppliers Association, 1980).

The particular gas constant R_I (J/(kg K)) of the gas stream is given by:

$$R_I = \frac{R_U}{M_{wi}} \quad (\text{B.3})$$

where R_U = universal gas constant (8314 J/(kmole K)).

Bell (1978) introduced a "double exponential" model for the blowdown of a pressurized pipeline:

$$\dot{m}_E = \frac{\Gamma \dot{m}_O}{(1 + \eta)} \left[\exp\left(-\frac{t}{\eta^2 \epsilon}\right) + \eta \exp\left(-\frac{t}{\epsilon}\right) \right] \quad (\text{B.4})$$

where:

- $\dot{m}_E$ = mass release rate (kg/s)
- $\dot{m}_O$ = initial gas release rate (kg/s) at time $t = 0$ s
- Γ = inertial delay factor (< 1.0)
- t = time after the release (s)
- $\eta = M_T / (\epsilon \Gamma \dot{m}_O)$ = mass conservation factor
- M_T = total mass to be released (kg)
- ϵ = time constant (s)

This model has been scaled so that the total mass to be released is recovered upon the following integration:

$$\int_0^\infty \dot{m}_E(t) dt = M_T \quad (\text{B.5})$$

The initial release rate $\dot{m}_O$ may be calculated from the adiabatic choked flow condition:

$$\dot{m}_O = \frac{P_O A_E \sqrt{k_E}}{\sqrt{R_E \bar{Z}_E T_O}} \left[\frac{2}{k_E + 1} \right]^{\frac{1}{2} \{ (k_E + 1) / (k_E - 1) \}} \quad (\text{B.6})$$

which may be found in any standard reference text on compressible flow (e.g., Shapiro, 1953). In this equation:

- P_O = gas pressure in pipeline before rupture (Pa)
- A_E = cross sectional area of rupture (m^2)
- k_E = ratio of specific heats for the pipeline gas (C_p / C_v)
- R_E = gas constant for the pipeline gas ($\text{J}/(\text{kg K})$)
- T_O = temperature of gas in pipeline before rupture (K)
- $\bar{Z}_E$ = gas compressibility at the exit (assumed to be 1.0)

and the time constant ϵ has been shown (Wilson, 1979) to be given by:

$$\epsilon = \frac{2}{3} \frac{l}{C_O} \left(\frac{k_E F l}{d} \right)^{1/2} \quad (\text{B.7})$$

where: l = pipeline length (m)
 C_o = speed of sound in pipeline gas before rupture (m/s)
 F = pipeline friction factor
 d = pipeline inside diameter (m)

The total mass released is determined by:

$$M_T = \frac{l_{EFF} A_E P_o}{R_E \bar{Z}_C T_o} \quad (B.8)$$

where: $\bar{Z}_C$ = pipeline gas compressibility prior to the rupture.

l_{EFF} = effective pipeline length to allow for the extra gas released during the time taken for the ESD valves to fully close.
 $= l \cdot (1 + \delta)$

The δ value represents the additional mass and is expressed as a fraction of the total mass of the gas contained in the isolated segment of the pipeline. Numerical modelling studies have shown that this excess can be of the order of 0.3 for a valve closure time of 30 s, a pipeline length of 1600 m, and a pipeline diameter of 15.5 cm (APIGEC, 1978). That is, the gas released to the atmosphere for this example is 1.3 times that contained within the 1600 m segment of the pipeline.

Sonic velocity in the pipeline gas is given by:

$$C_o \equiv \sqrt{k_E R_E \bar{Z}_C T_o} \quad (B.9)$$

The expression for the initial mass rate (Equation B.6) is based on adiabatic choked flow theory. At the onset of a pipeline rupture, an expansion wave travels down the pipeline at the local speed of sound. At the rupture exit, the gas flow behind the wave accelerates to sonic velocity. Typically, the region of significant gas acceleration is confined to a length of pipeline approximately 200 diameters upstream of the rupture point. This region of the flow is assumed to be determined by an adiabatic process in which the sum of the internal and kinetic energies of the flow remains constant.

Beyond approximately 200 diameters upstream of the rupture point, the gas flow is characterized by a relatively small change in gas velocity. This, coupled with the fact that most sour gas pipelines are buried in the ground which acts as a thermal reservoir, indicates that much of the pipeline during the entire blowdown time is undergoing an isothermal process. For most of the blowdown time for almost all the pipeline length, the pipeline is releasing gas as a fixed volume isothermal (decreasing pressure) containment vessel. The expression for the time constant (Equation B.7) is based on isothermal flow theory.

The preceeding two paragraphs justify adopting adiabatic assumptions near the exit section of the pipeline ($\bar{Z}_E = 1.0$) and isothermal assumptions away from the exit section of the pipeline.

The double exponential mass release model has been tested against the experiments of Dielwart *et al.* (1979) by Wilson (1981) and subsequently used by Choukalos (1982) in the Alberta Environment risk model. Its use is based on two important considerations:

- An exponential decay in mass flow is the exact solution to an isothermal fixed length blowdown after the rupture expansion wave reaches the pipeline ESD valve.
- The satisfactory agreement of the model with the release rate time history measured in a study conducted by APIGEC (Dielwart *et al.*, 1979). Wilson (1981) found the best agreement using $\Gamma = 0.5$ in the double exponential relation.

In the light of the above considerations, the double exponential model of Bell (1978) and Wilson (1981) has been selected for implementation in this work.

B1.1.3 Continuous Pipeline Release

If a pipeline were to rupture and the ESD valve(s) between the ruptured segment and the well were to fail, the release of the sour gas would be characterized by an initial transient peak which would decay to a steady state value. In this event, the mass release rate is approximated by:

$$\dot{m}_E(t) = \text{MAX}[\dot{m}_{E,T}(t), \dot{m}_{E,S}] \quad (\text{B.10})$$

where $\dot{m}_{E,T}(t)$ is the transient mass release rate and $\dot{m}_{E,S}$ is the steady state mass release rate.

The mass release profile represented by the above equation is a continuous profile which decays exponentially to time t_s and is constant thereafter. The time t_s is given by the solution to the equation:

$$\frac{\Gamma \dot{m}_O}{(1 + \eta)} \left[\exp\left(-\frac{t_s}{\eta^2 \epsilon}\right) + \eta \exp\left(-\frac{t_s}{\epsilon}\right) \right] = \dot{m}_{E,S} \quad (\text{B.11})$$

B1.2 Jet Expansion Module

Throughout a well blowout, and for virtually the entire duration of a pipeline blowdown, the discharging gas experiences choked flow conditions at the rupture exit. The expansion of the gas from the sonic, underexpanded state to atmospheric pressure, the entrainment of ambient air, the influence of drag, and the potential combustion of gas are treated in the jet expansion module as a series of simplified processes. The parameterization of these processes required extensive review of existing methods and the development of practical working equations from basic principles. This effort constituted original model development specifically undertaken for the present model.

Figure B.2 shows the exit of a gas jet at sonic velocity from an opening ("E"). The jet undergoes an adiabatic expansion due to the equalization of the exit pressure to atmospheric pressure ("Q"). Air entrainment and drag cause a deceleration of the jet to sub-sonic velocity ("S"). The possible ignition of the jet causes the creation of combustion products and the generation of heat which raises the jet temperature ("C").

A major assumption in the above view of the jet expansion process is that the four "regions" may be modelled as series processes, rather than simultaneous processes. In addition to this, a further assumption is made that the jet may be treated in a one-dimensional, quasi-steady fashion.

B1.2.1 Stagnation Zone

At the exit, or rupture, there are certain known quantities which may be regarded as inputs:

- M_{WE} = molecular weight of the discharging gas at "E" (kg/kmole).
- C_{PE} = specific heat at constant pressure of the gas at "E" (J/(kg K)).
- T_O = stagnation temperature of the gas before discharge (K)
- A_E = area of the exit or rupture (m^2)
- $\dot{m}_E$ = the mass flow rate of gas discharge (kg/s)
- R_E = particular gas constant of the discharging gas (J/(kg K))

The ratio of specific heats for the discharging gas is, from the definition:

$$k_E \equiv \frac{C_{PE}}{C_{VE}} = \frac{C_{PE}}{C_{PE} - R_E} \quad (B.12)$$

From Shapiro (1953) the pressure at the exit of an adiabatic choked flow discharge is given by:

$$P_E = \frac{\dot{m}_E}{A_E} \left[\frac{R_E T_O}{k_E} \left(\frac{2}{k_E + 1} \right) \right]^{1/2} \quad (B.13)$$

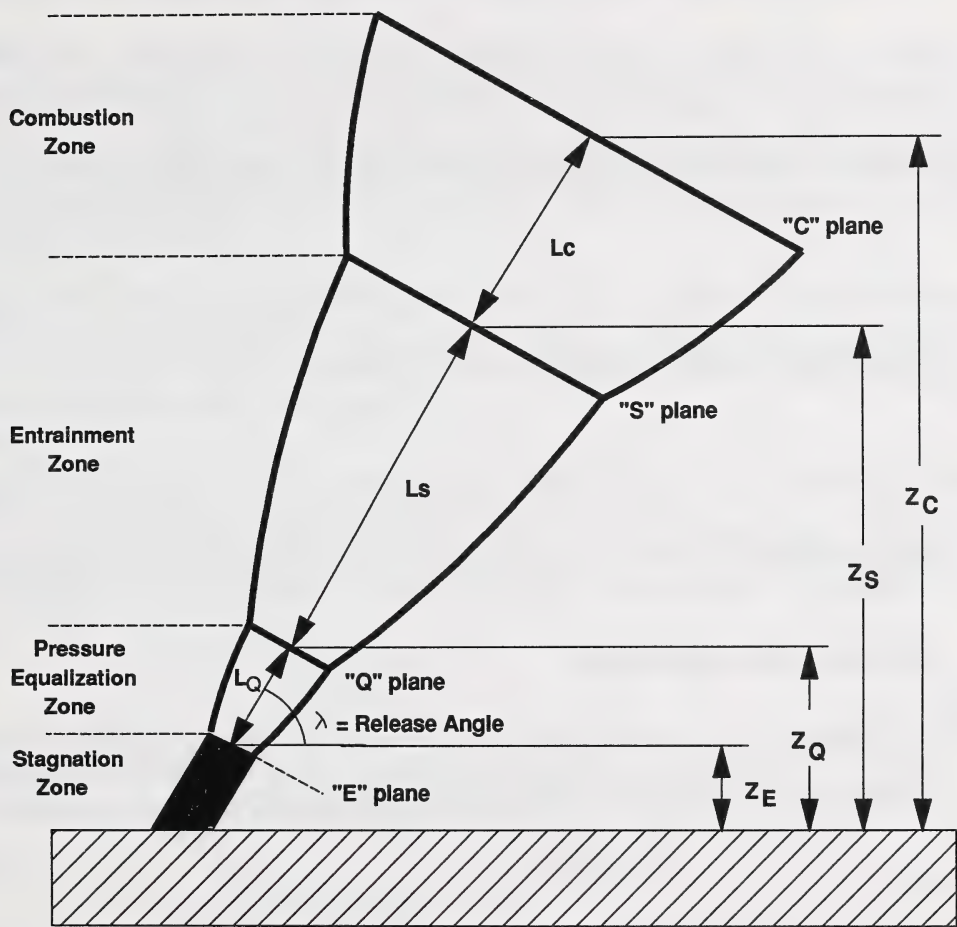


FIGURE B.2
Jet Expansion Region.

The choked flow condition constrains the exit velocity (V_E) to be sonic:

$$V_E = \left[k_E R_E T_O \left(\frac{2}{k_E + 1} \right) \right]^{1/2} \quad (\text{B.14})$$

By conservation of mass, the gas density at the exit may be determined:

$$\rho_E = \frac{\dot{m}_E}{A_E V_E} \quad (\text{B.15})$$

The ideal gas law requires the gas temperature at the exit to be:

$$T_E = \frac{P_E}{\rho_E R_E} \quad (\text{B.16})$$

The conditions at the exit P_E , V_E , ρ_E and T_E can therefore be defined from the preceding relationships.

Subsonic Flow Conditions

As the pressure at "E" approaches atmospheric pressure, the choked flow assumption at the rupture is not valid. In this event, which can occur for small leaks or for transient mass discharges at large times, the conditions at the "E" plane are given as:

$$P_E = P_A \quad (\text{B.17})$$

$$T_E = \left\{ -C_{PE} + \left[C_{PE}^2 + \frac{2C_{PE}T_O \dot{m}_E^2 R_E^2}{A_E^2 P_A^2} \right]^{1/2} \right\} \frac{A_E^2 P_A^2}{\dot{m}_E^2 R_E^2} \quad (\text{B.18})$$

$$\rho_E = \frac{P_A}{R_E T_E} \quad (\text{B.19})$$

$$V_E = \frac{\dot{m}_E}{\rho_E A_E} \quad (\text{B.20})$$

The equation for P_E assumes no significant pressure deficit to occur at the rupture. It is worthy of note that the expression for T_E is derived from the energy balance:

$$\dot{m}_E C_{PE} T_O = \dot{m}_E C_{PE} T_E + \frac{\dot{m}_E V_E^2}{2} \quad (\text{B.21})$$

B1.2.2 Pressure Equalization Zone

Birch *et al.* (1984) studied the behavior of underexpanded compressible sonic jets of natural gas into quiescent air. They predicted the concentration field arising from the expansion of these jets by treating them as classical sub-sonic jets with an appropriate length scale called the "pseudo-diameter". The pseudo-diameter is a theoretical concept describing the effective size of the jet source, which when substituted into the equations defining a sub-sonic round jet, adequately describes the behavior of the jet flow. Their predictions compared favourably with experimental data.

The area of the jet at the "Q" plane (A_Q) shown in Figure B.2 is given by the circular area defined by the pseudo-diameter. Specifically, the condition of the jet at the "Q" plane arises from the consideration of the area that would be occupied by the same mass flow as at the exit plane (the "E" plane), at the same temperature as that at the exit plane, at ambient pressure and at uniform sonic velocity.

At the exit conditions (the "E" plane), the gas jet is considered to be "underexpanded" since the exit pressure may exceed atmospheric (ambient) pressure by an order of magnitude or so. As the jet pressure equilibrates to atmospheric pressure, the jet expands. At "Q" in Figure B.2, the jet has undergone no changes in composition, nor significant change in temperature. At the "Q" plane one can define the following conditions:

$$\begin{aligned} M_{wQ} &= M_{wE} \\ C_{PQ} &= C_{PE} \\ R_Q &= R_E \\ k_Q &= k_E \end{aligned} \quad (B.22)$$

Continuity of mass (i.e. no entrainment) demands that:

$$A_Q = A_E \frac{\rho_E V_E}{\rho_Q V_Q} \quad (B.23)$$

Following the procedure of Birch *et al.* (1984), the jet velocity at "Q" may be considered sonic when the jet pressure has decayed to the ambient value:

$$V_Q = C_Q \equiv \sqrt{k_Q R_Q T_Q} \quad (B.24)$$

At "Q" the ideal gas law is applied:

$$\rho_A = \frac{P_A}{R_Q T_Q} \quad (B.25)$$

where $P_Q = P_A$ (ambient surface pressure) has been applied.

Assuming adiabatic conditions, the application of the conservation of energy between the "Q" plane and the stagnation conditions at "E" gives:

$$T_Q = \frac{2T_o}{k_Q + 1} \quad (\text{B.26})$$

It can be shown that $T_Q = T_E$, given the relationship for T_E in Section B1.2.1.

The above equations form a closed set of equations for the four unknowns A_Q , V_Q , ρ_Q and T_Q . Thus, the conditions at the "Q" plane where the underexpanded jet at the exit is expanded to atmospheric pressure can be estimated. The length of the pressure equalization zone (L_Q) is expected to be of the order of a few pipe diameters and is neglected in estimating the height of the plume above the ground.

Subsonic Flow Conditions

The sonic velocity of the flow at "E" may be calculated from:

$$C_E \equiv \sqrt{k_E R_E T_E} \quad (\text{B.27})$$

If $V_E \geq 0.3C_E$, then the flow must be considered compressible. However, since $P_E = P_A$ has been assumed, no pressure equalization stage is required, the "Q" plane calculations may be skipped and:

$$\begin{aligned} P_Q &= P_E \\ T_Q &= T_E \\ V_Q &= V_E \\ \dot{m}_Q &= \dot{m}_E \\ A_Q &= A_E \end{aligned} \quad (\text{B.28})$$

B1.2.3 Entrainment Zone

It is clear that sonic velocity cannot persist for long in the jet as ambient air entrainment and obstacles to the flow cause the jet to decelerate. At "Q" in Figure B.2, the discharged gas has not changed in composition from the stagnation composition. As air is entrained into the jet, however, the molecular weight and the specific heat at constant pressure for the gas-air mixture changes (assuming steady state conditions):

$$M_{ws} = \frac{M_{WA} M_{WQ}}{M_{WQ}(\dot{m}_A/\dot{m}_S) + (1 - \dot{m}_A/\dot{m}_S)M_{WA}} \quad (\text{B.29})$$

$$C_{PS} = \left(\frac{\dot{m}_A}{\dot{m}_S} \right) C_{PA} + \left(1 - \frac{\dot{m}_A}{\dot{m}_S} \right) C_{PQ} \quad (\text{B.30})$$

where: M_{WA} = molecular weight of air (28.95 kg/kmole)
 C_{PA} = specific heat at constant pressure for air (997 J/(kg K))
 $\dot{m}_A$ = mass flow of air entrained between "Q" plane and "S" plane (kg/s)
 $\dot{m}_S$ = mass flow of gas-air mixture through the "S" plane (kg/s)

The ratio of specific heats for the gas-air mixture is, by definition:

$$k_s = \frac{C_{PS}}{C_{PS} - R_s} \quad (B.31)$$

where R_s = particular gas constant for the gas-air mixture at the "S" plane.

Conservation of mass from the "Q" plane to the "S" plane demands that:

$$\dot{m}_S = \dot{m}_E + \dot{m}_A = \rho_s A_s V_s \quad (B.32)$$

where $\dot{m}_E = \dot{m}_Q$ has been applied. The conservation of energy for an adiabatic process between "Q" and "S" gives:

$$\dot{m}_E C_{PQ} T_Q + \dot{m}_E \frac{V_Q^2}{2} + \dot{m}_A C_{PA} T_A = \dot{m}_S C_{PS} T_S + \dot{m}_S \frac{V_S^2}{2} \quad (B.33)$$

where T_A = ambient surface temperature (K) and where the kinetic energy of entrained air, the potential energy and the work against drag have been neglected.

The conservation of momentum dictates that:

$$\dot{m}_E V_Q + \dot{m}_A U_Q \cos \lambda = \dot{m}_S V_S + \frac{C_{D1}}{2} \left(\dot{m}_E + \frac{\dot{m}_A}{2} \right) \left(\frac{V_Q + V_S}{2} \right) \quad (B.34)$$

where: U_Q = ambient wind speed at height "Q" (m/s)
 λ = angle of jet with horizontal
 C_{D1} = drag coefficient
= 0 for a jet, and
= 1 for a cloud

The above conservation of momentum equation assumes an average velocity between the "Q" and the "S" planes in the estimation of drag force.

The ideal gas law applied at "S" results in:

$$\rho_s = \frac{P_A}{R_s T_s} \quad (B.35)$$

The jet velocity at "S", in terms of the Mach number (M_s) is:

$$V_s = M_s \sqrt{k_s R_s T_s} \quad (\text{B.36})$$

The previous equations represent a closed set of equations for all the variables at "S" and $\dot{m}_A$, provided the Mach number M_s is specified. It is reasonable to choose M_s small enough so that flow compressibility effects become small:

$$\begin{aligned} M_s &\sim 0.3 && \text{for a jet} \\ &\sim 0.01 && \text{for a cloud} \end{aligned} \quad (\text{B.37})$$

Due to the non-linear and coupled nature of these governing equations, the solution of the equation set is best handled iteratively through the method given in Table B.2.

Once all the relevant variables at "S" are known, it becomes possible to estimate the length of the jet between the "Q" and "S" plane in Figure B.2:

[EQUATION]

(B.38)

where: L_s = jet length between "Q" and "S" plane (m)
 ρ_A = ambient air density (kg/m^3)
 α = entrainment constant = 0.13

Equation B.38 has employed the Taylor hypothesis for jet entrainment:

$$\dot{m}_A = \alpha \rho_A A_{EFF} V_{EFF} \quad (\text{B.39})$$

Table B.2
Estimation of "S" Plane Parameters

The procedure may be summarized as follows:

- (1) Assume a value for the entrained mass rate $\dot{m}_A$.
- (2) Calculate $\dot{m}_S$ since $\dot{m}_e$ is known (Equation B.32).
- (3) Calculate M_{wS} (Equation B.29).
- (4) Calculate C_{pS} (Equation B.30).
- (5) Calculate R_S (Equation B.3).
- (6) Calculate k_S (Equation B.31).
- (7) Calculate V_S (Equation B.33 with Equation B.36 for T_S).
- (8) Calculate T_S (Equation B.36).
- (9) Calculate ρ_S (Equation B.35).
- (10) Calculate A_S (Equation B.32).
- (11) Calculate the difference between the left-hand side and the right-hand side of the conservation of momentum equation (Equation B.34).
- (12) As long as the difference calculated in step (11) is significantly different from zero, revise the value for $\dot{m}_A$ and go back to step (2). If the residual is small enough (< 0.01 kg/s), terminate the iteration.

This procedure may be treated as a root-finding problem for the residual calculated in step (11) versus the entrained air mass rate $\dot{m}_A$.

where V_{EFF} = effective tangential velocity difference (m/s)

$$V_{EFF} = \frac{\left[\dot{m}_E - \frac{\dot{m}_A}{\left(\frac{A_S}{A_Q} \right)^{1/2} - 1} \right] \ln \left(\frac{A_S}{A_Q} \right) + 2\dot{m}_A}{\left(\frac{\rho_Q + \rho_A}{2} \right) (A_S - A_Q)} - U_Q \cos \lambda \quad (B.40)$$

and A_{EFF} = effective surface area between "Q" and "S" (m^2).

$$A_{EFF} = L_S \sqrt{\pi (A_S^{1/2} + A_Q^{1/2})} \quad (B.41)$$

The expression for A_{EFF} assumes the region between the "Q" plane and the "S" plane can be approximated by a conical volume.

Finally, the elevation of the "S"-plane above the ground is:

$$Z_S = Z_E + L_S \sin \lambda \quad (B.42)$$

where Z_E = elevation of the rupture point "E" in Figure B.2. Note that the length of the pressure equalization zone (L_Q) has been ignored since $L_S \gg L_Q$.

Subsonic Flow Conditions

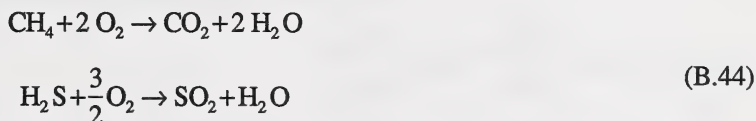
If $V_E < 0.3 C_E$, then the flow can be considered incompressible and there is no need to consider either the pressure equalization or flow deceleration calculation, and both the "Q" plane and "S" plane calculations (Sections B1.2.2 and B1.2.3) may be skipped and:

$$\begin{aligned} P_S &= P_E \\ T_S &= T_E \\ V_S &= V_E \\ \dot{m}_Q &= \dot{m}_E \\ A_S &= A_E \end{aligned} \quad (B.43)$$

B1.2.4 Combustion Zone

In the event that the gas-air mixture is ignited, as could be the case for an uncontrolled release of sour gas, the chemical transformation of the gas-air jet upon combustion and the increase in jet temperature due to the heat of combustion must be modelled.

Assuming the chief components of sour gas to be methane (CH₄), hydrogen sulphide (H₂S) and carbon dioxide (CO₂) and the components of air to be nitrogen (N₂ : 79% by volume; 76.8 % by mass) and oxygen (O₂ : 21% by volume; 23.2% by mass), the primary combustion reactions of interest are:



Here, complete stoichiometric combustion of H₂S and CH₄ is assumed in the region between "S" and "C" as shown in Figure B.2.

The molecular weight of the combusted gas and air mixture at "C" depends on the mass flow of the various species at the "C" plane:

[EQUATION] (B.45)

where:

- $M_{w\text{CO}_2}$ = molecular weight of CO₂ = 44 kg/kmole
- $M_{w\text{SO}_2}$ = molecular weight of SO₂ = 64 kg/kmole
- $M_{w\text{H}_2\text{O}}$ = molecular weight of H₂O = 18 kg/kmole
- $M_{w\text{N}_2}$ = molecular weight of N₂ = 28 kg/kmole
- $M_{w\text{O}_2}$ = molecular weight of O₂ = 32 kg/kmole
- M_{wc} = molecular weight of combusted gas air mixture at "C"
(kg/kmole)
- $\dot{m}_c$ = mass flow of combusted gas and air at "C" (kg/s)
- $(\dot{m}_c)_{\text{CO}_2}$ = mass flow of CO₂ at "C" (kg/s)
- $(\dot{m}_c)_{\text{SO}_2}$ = mass flow of SO₂ at "C" (kg/s)
- $(\dot{m}_c)_{\text{H}_2\text{O}}$ = mass flow of H₂O at "C" (kg/s)
- $(\dot{m}_c)_{\text{N}_2}$ = mass flow of N₂ at "C" (kg/s)
- $(\dot{m}_c)_{\text{O}_2}$ = mass flow of O₂ at "C" (kg/s)

The mass flows of the various species depend on the mass fractions of CH₄, H₂S and CO₂ in the sour gas at "S", the mass flow of sour gas at "S", the total mass flow (sour gas and air) at "S", and the mass flow of air entrained between "S" and "C":

$$(\dot{m}_C)_{\text{CO}_2} = a\dot{m}_E \frac{M_{\text{WCO}_2}}{M_{\text{WCH}_4}} + (1 - a - b)\dot{m}_E \quad (\text{B.46})$$

$$(\dot{m}_C)_{\text{SO}_2} = b\dot{m}_E \frac{M_{\text{WSO}_2}}{M_{\text{WH}_2\text{S}}} \quad (\text{B.47})$$

$$(\dot{m}_C)_{\text{H}_2\text{O}} = 2a\dot{m}_E \frac{M_{\text{WH}_2\text{O}}}{M_{\text{WCH}_4}} + b\dot{m}_E \frac{M_{\text{WH}_2\text{O}}}{M_{\text{WH}_2\text{S}}} \quad (\text{B.48})$$

$$(\dot{m}_C)_{\text{N}_2} = 0.768(\dot{m}_S - \dot{m}_E) + 0.768\dot{m}_{\text{AC}} \quad (\text{B.49})$$

$$(\dot{m}_C)_{\text{O}_2} = 0.232(\dot{m}_S - \dot{m}_E) + 0.232\dot{m}_{\text{AC}} - 2a\dot{m}_E \frac{M_{\text{WO}_2}}{M_{\text{WCH}_4}} - \frac{3}{2}b\dot{m}_E \frac{M_{\text{WO}_2}}{M_{\text{WH}_2\text{S}}} \quad (\text{B.50})$$

where: a = mass fraction CH₄ in sour gas
 b = mass fraction H₂S in sour gas
 $(1-a-b)$ = mass fraction CO₂ in sour gas
 $\dot{m}_S$ = mass flow of sour gas and air at "S" (kg/s)
 $\dot{m}_E$ = mass flow of sour gas at "E" (kg/s)
 $\dot{m}_{\text{AC}}$ = mass flow of air entrained between "S" and "C" (kg/s)

Similarly, the relation for the specific heat at constant pressure at "C" is:

$$[\text{EQUATION}] \quad (\text{B.51})$$

where the specific heats at constant pressure (C_p) can be temperature dependent functions (Himmelblau, 1974):

$$C_{p\text{CO}_2} = \frac{4184}{44} [6.393 + 1.01 \cdot 10^{-2}T_c - 3.405 \cdot 10^{-6}T_c^2] \quad (\text{B.52})$$

$$C_{p\text{SO}_2} = \frac{4184}{64} [9.299 + 9.33 \cdot 10^{-3}(T_c - 273) - 7.418 \cdot 10^{-6}(T_c - 273)^2 + 2.057 \cdot 10^{-9}(T_c - 273)^3] \quad (\text{B.53})$$

$$C_{p\text{H}_2\text{O}} = \frac{4184}{18} [6.970 + 3.464 \cdot 10^{-3}T_c - 4.83 \cdot 10^{-7}T_c^2] \quad (\text{B.54})$$

$$C_{p_{N_2}} = \frac{4184}{28} [6.529 + 1.488 \cdot 10^{-3} T_C - 2.271 \cdot 10^{-7} T_C^2] \quad (B.55)$$

$$C_{p_{O_2}} = \frac{4184}{32} [6.732 + 1.505 \cdot 10^{-3} T_C - 1.791 \cdot 10^{-7} T_C^2] \quad (B.56)$$

In the above equations, the specific heats at constant pressure are expressed in units of J/(kg K).

It follows from the expressions for M_{WC} and for C_{PC} , that:

$$k_C = \frac{C_{PC}}{C_{PC} - R_C} \quad (B.57)$$

where R_C = particular gas constant of the combusted gas air mixture at the "C" plane.

These properties of the combusted gas-air mixture at "C" depend on two unknown quantities: $\dot{m}_{AC}$ and T_C . These quantities, and others will be determined by the application of conservation laws in the region between "S" and "C" in Figure B.2. Conservation of mass dictates that:

$$\dot{m}_C = \dot{m}_S + \dot{m}_{AC} = \rho_C A_C V_C \quad (B.58)$$

where: ρ_C = density of the combusted gas air mixture at "C" (kg/m³)
 A_C = cross-sectional area of the plume at "C" (m²)
 V_C = velocity of the combusted gas air mixture at "C" (m/s)

Conservation of energy gives:

$$\dot{m}_S C_{PS} T_S + \dot{m}_S \frac{V_S^2}{2} + Q_H \left[\frac{\dot{m}_E}{\rho_{EO}} (1 - f_R) \right] + \dot{m}_{AC} C_{PA} T_A = \dot{m}_C C_{PC} T_C + \dot{m}_C \frac{V_C^2}{2} \quad (B.59)$$

where: T_A = ambient surface temperature (K)
 C_{PA} = specific heat at constant pressure for ambient air (997 J/(kg K))
 Q_H = heat produced by the combustion reaction (J/m³)
 f_R = fraction of heat produced by combustion which is lost by radiation = 0.25 (Alberta Environment, 1980).
 ρ_{EO} = density of sour gas at standard conditions of 15 °C and 101.3 kPa

The heat produced by the combustion reaction is given by Alberta Environment (1980) in terms of low heat values for the components of sour gas. Thus, when the low heat value for the escaping sour gas is multiplied by the volume flow rate of sour gas exiting the rupture at the standard conditions ($\dot{m}_E / \rho_{EO}$), the rate of heat input to the jet (in J/s) is obtained.

The conservation of momentum provides another governing equation:

$$\dot{m}_S V_S + \dot{m}_{AC} U_C \cos \lambda = \dot{m}_C V_C \quad (\text{B.60})$$

where: U_C = ambient wind speed at height "C" (m/s)
 λ = angle of jet with horizontal

The ideal gas law is another constraint on the "C" plane:

$$\rho_C = \frac{P_A}{R_C T_C} \quad (\text{B.61})$$

where P_A = surface air pressure (Pa).

For a jet, the same air entrainment model as was used at the "S" plane in Section B1.2.3 is utilized at the "C" plane:

$$\dot{m}_{AC} = \alpha \sqrt{\pi} \rho_A L_C (A_S^{1/2} + A_C^{1/2}) V_{EFF} \quad (\text{B.62})$$

$$V_{EFF} = \frac{\left[\dot{m}_S - \frac{\dot{m}_{AC}}{\left(\frac{A_S}{A_C} \right)^{1/2} - 1} \right] \ln \left(\frac{A_C}{A_S} \right) + 2\dot{m}_{AC}}{\left(\frac{\rho_S + \rho_A}{2} \right) (A_C - A_S)} - U_S \cos \lambda \quad (\text{B.63})$$

L_C = distance between the "S" plane and the "C" plane in Figure B.2 (m)
 α = entrainment constant = 0.13
 ρ_A = ambient air density (kg/m³)
 U_S = wind speed at "S"

The length L_C can be estimated from a parameterization by Craven (1972):

$$L_C = \frac{10.6}{c_T} \left\{ \frac{A_E T_C}{\pi T_E a_T} \left[c_T + (1 - c_T) \frac{M_{WA}}{M_{WE}} \right] \right\}^{1/2} - L_S \quad (\text{B.64})$$

where: A_E = area of rupture (m²)
 c_T = molar concentration of fuel in the stoichiometric mixture
 a_T = molar ratio of reactants to products
 M_{WA} = molecular weight of standard air (28.95 kg/kmole)
 M_{WE} = molecular weight of sour gas at rupture (kg/kmole)
 L_S = length between "Q" and "S" planes in Figure B.2
 L_C = length between "S" and "C" planes in Figure B.2
 T_C = Temperature of combusted gas - air mixture at "C" (K)
 T_E = temperature of sour gas at rupture (K)

The calculation of c_T and a_T proceeds as follows:

$$V_{\text{CO}_2} = 1 - V_{\text{H}_2\text{S}} - V_{\text{CH}_4} \quad (\text{B.65})$$

where: V_{CO_2} = volume fraction CO_2 in the escaping gas

$V_{\text{H}_2\text{S}}$ = volume fraction H_2S in the escaping gas

V_{CH_4} = volume fraction of CH_4 in the escaping gas

$$a_T = \frac{1 + 4.76(2V_{\text{CH}_4} + 1.5V_{\text{H}_2\text{S}})}{3V_{\text{CH}_4} + 2V_{\text{H}_2\text{S}} + V_{\text{CO}_2} + 3.76(2V_{\text{CH}_4} + 1.5V_{\text{H}_2\text{S}})} \quad (\text{B.66})$$

$$c_T = \frac{1}{1 + 4.76(2V_{\text{CH}_4} + 1.5V_{\text{H}_2\text{S}})} \quad (\text{B.67})$$

The previous equations form a closed system of equations for all the unknowns at the "C" plane. The solution procedure for this equation set is very similar to that employed in Section B1.2.3 and is given in Table B.3.

Table B.3

Estimation of "C" Plane Parameters for a Jet.

The procedure may be summarized as follows:

- (1) Assume an entrained mass rate $\dot{m}_{AC}$.
- (2) Assume $T_C = T_A$.
- (3) Calculate $\dot{m}_C$ since $\dot{m}_s$ is known (Equation B.58).
- (4) Calculate V_C (Equation B.60).
- (5) Calculate M_{WC} from Equation B.45 knowing all the species mass flows (Equations B.46 to B.50).
- (6) Calculate R_C (Equation B.3).
- (7) Calculate C_{PC} (Equation B.51). The species mass flows are known from Equations B.46 to B.50.
- (8) Calculate ρ_C (Equation B.61).
- (9) Calculate A_C (Equation B.58).
- (10) Calculate L_C (Equation B.64).
- (11) Calculate the residual (left-hand side minus right-hand side) of the air entrainment model equation (Equation B.62).
- (12) As long as the residual calculated in step (11) is significantly different from zero, revise the value of $\dot{m}_{AC}$ and go back to step (3). If the residual is small enough ($< 0.1\%$), proceed with step (13). If step (13) has been performed four times then terminate the iteration.
- (13) Update T_C using Equation B.59 and go back to step (3). Four updates for T_C are sufficient to give a convergent solution set.

This procedure may be treated as a root-finding problem for the residual calculated in step (11) versus the entrained air mass rate $\dot{m}_{AC}$.

For a cloud, however, an alternate approach was adopted since the air entrainment model (Equation B.62) is not valid and may lead to incomplete combustion. Under these conditions, sufficient air for complete combustion is ensured by forcing $\dot{m}_{AC}$, the mass flow of air entrained between "S" and "C", to be larger than or equal to the $\dot{m}_{AC}$ solved from Equation B.50 when $(\dot{m}_C)_{O_2}$ is set to zero. Secondly, the cloud is assumed to grow according to:

$$\sigma_C = (\sigma_s^2 + \sigma^2)^{1/2} \quad (B.68)$$

where: σ_C is the standard deviation of the plume spread at the "C" plane.
 σ_s represents the "initial dilution" at the "S" plane and is estimated from:

$$\sqrt{\frac{A_s}{\pi}} \sim 2\sigma_s$$

σ represents the growth rate of the plume between the "S" and "C" planes due to atmospheric and combustion generated turbulence.

Combustion generated turbulence is difficult to estimate and for the purposes of the ensuring analysis, is conservatively neglected. The growth due to atmospheric turbulence is estimated from:

$$\sigma = \sigma_{PS} = S_{REF} L_C^{P_Y} \quad (B.69)$$

where σ_{PS} is the Pasquill-Smith horizontal plume spread. The constants S_{REF} and P_Y are the same as those by Alberta Environment for passive dispersion. These constants depend on atmospheric stability and surface roughness. The values given in Table B.4 correspond to a surface roughness Z_o of 0.1 m.

Table B.4

Stability Dependent Parameters Used to Estimate "C" Plane Parameters for a Cloud.

	Unstable	Neutral	Stable
S_{REF}	0.367	0.156	0.077
P_Y	0.88	0.88	0.88

By assuming the radius of the plume at "C" to equal twice the standard deviation σ_C , the area of the plume A_C at "C" can be estimated by substitution into Equation B.68:

$$A_C = 4\pi \left(\frac{R_S^2}{4} + S_{REF}^2 L_C^{2P_Y} \right) \quad (B.70)$$

The length L_C is estimated from the following correlation for a buoyant cloud (Brzustowski, 1973):

$$L_C = 2\sqrt{\frac{A_S}{\pi}} \left\{ 2.96 \left(\frac{\rho_S}{\rho_A} \right)^{1/2} (F_{RS})^{1/5} \left(\frac{\dot{m}_E}{\dot{m}_S} \right)^{3/5} \left[1 + \frac{M_{WA}}{M_{WE}} \left(\frac{1}{0.297 C_L} - 1 \right) \right]^{3/5} \right\} - L_S \quad (B.71)$$

where:

$$F_{RS} = \frac{V_S^2}{2g\sqrt{\frac{A_S}{\pi}}} \left(\frac{\rho_A}{\rho_S} \right)^{1/2} \frac{C_{PA} T_A}{\frac{\dot{m}_E}{\dot{m}_S} Q_H + C_{PS}(T_S - T_A)}$$

$$C_L = \left\{ \frac{V_{H_2S}}{(V_{H_2S} + V_{CH_4})C_{L(H_2S)}} + \frac{V_{CH_4}}{(V_{H_2S} + V_{CH_4})C_{L(CH_4)}} \right\}^{-1}$$

ρ_C = density of the combusted gas air mixture at "S" (kg/m³)

ρ_A = density of the ambient air (kg/m³)

M_{WA} = molecular weight of air (28.95 kg/kmole)

M_{WE} = molecular weight of sour gas at rupture (kg/kmole)

$C_{L(H_2S)}$ = H₂S concentration at the lean flammability limit, fraction by volume (0.042)

$C_{L(CH_4)}$ = CH₄ concentration at the lean flammability limit, fraction by volume (0.05)

V_S = velocity of the combusted gas air mixture at "S"

g = acceleration due to gravity (m/s²)

C_{PA} = specific heat at constant pressure for ambient air (997 J/(kg K))

T_A = ambient surface temperature (K)

Q_H = heat produced by the combustion reaction (J/m³)

C_{PS} = specific heat at constant pressure of the gas-air mixture at "S" plane (J/(kg K))

T_C = temperature of the combusted gas-air mixture at "C" plane (K)

Combining Equations B.70 and B.71 with the conservation of mass equation (Equation B.58) and the ideal gas law (Equation B.61), the mass of air entrained is estimated from:

$$\dot{m}_{AC} = -\dot{m}_s + \frac{V_C P_A A_C}{R_C T_C} \quad (\text{B.72})$$

With Equations B.71 and B.72 replacing Equations B.64 and B.62, a closed system of equations for all unknowns at the "C" plane for the ignited cloud case can be formed. The solution procedure for this equation set is given in Table B.5.

Once all the variables at "C" are known, several important additional parameters may be calculated. The mass flow of air at "C" may be estimated by:

$$(\dot{m}_A)_C = \frac{(\dot{m}_C)_{O_2}}{0.232} \quad (\text{B.73})$$

The mass flow of combusted gas at "C" is hence given by:

$$(\dot{m}_E)_C = \dot{m}_C - (\dot{m}_A)_C \quad (\text{B.74})$$

The properties of combusted gas at "C" are required for subsequent dispersion calculations:

$$(C_{PE})_C = \frac{\dot{m}_C C_{PC} - (\dot{m}_A)_C C_{PA}}{(\dot{m}_E)_C} \quad (\text{B.75})$$

$$(R_E)_C = \frac{\dot{m}_C R_C - (\dot{m}_A)_C R_A}{(\dot{m}_E)_C} \quad (\text{B.76})$$

$$(M_{WE})_C = \frac{R_U}{(R_E)_C} \quad (\text{B.77})$$

where: R_U = universal gas constant (8314 J/(kg K))
 R_A = particular gas constant for air (287 J/(kmole kg))
 C_{PA} = specific heat at constant pressure for air (997 J/(kg K))

The concentration of SO₂ in the combusted gas at "C" is important since this gas replaces H₂S as the toxic component in the gas discharge:

$$(C_{SO_2})_C = \frac{(\dot{m}_C)_{SO_2}}{(\dot{m}_E)_C} (C_E)_C \quad (\text{B.78})$$

Table B.5

Estimation of "C" Plane Parameters for a Cloud.

The procedure may be summarized as follows:

- (1) Assume an entrained mass rate $\dot{m}_{AC}$.
- (2) Assume $T_C = T_A$.
- (3) Calculate $\dot{m}_C$ since $\dot{m}_S$ is known (Equation B.58).
- (4) Calculate V_C (Equation B.60).
- (5) Calculate M_{WC} from Equation B.45 knowing all the species mass flows (Equations B.46 to B.50).
- (6) Calculate R_C (Equation B.3).
- (7) Calculate C_{PC} (Equation B.51). The species mass flows are known from Equations B.46 to B.50.
- (8) Calculate ρ_C (Equation B.61).
- (9) Calculate A_C (Equation B.70).
- (10) Calculate L_C (Equation B.71).
- (11) Calculate the residual (left-hand side minus right-hand side) of the air entrainment model equation (Equation B.72).
- (12) As long as the residual calculated in step (11) is significantly different from zero, revise the value of $\dot{m}_{AC}$ and go back to step (3). If the residual is small enough ($< 0.1\%$), proceed with step (13). If step (13) has been performed four times then terminate the iteration.
- (13) Update T_C using Equation B.59 and go back to step (3). Four updates for T_C are sufficient to give a convergent solution set.

This procedure may be treated as a root-finding problem for the residual calculated in step (11) versus the entrained air mass rate $\dot{m}_{AC}$.

Where $(C_E)_C$, the concentration of combusted gas in the gas-air mixture at "C", is:

$$(C_E)_C = \frac{(\dot{m}_E)_C}{\dot{m}_C} \rho_C \quad (\text{B.79})$$

Finally, the elevation of the "C" plane above the rupture point is:

$$Z_C = Z_S + L_C \sin \lambda \quad (\text{B.80})$$

where: Z_C = elevation of the "S" plane in Figure B.2

Note that the length of the pressure equalization zone (L_Q) has been ignored since $L_C \gg L_Q$.

B1.3 Plume Rise Module

Once the expanded jet leaves ground level, the momentum and buoyancy of the jet will influence its rise until, at the point of final rise, atmospheric dispersion becomes the predominant transport mechanism. While momentum dominates immediately after jet expansion and jet-like behavior results, eventually buoyancy becomes an important factor and plume-like behavior results. Following the treatment of Wilson (1985), and consistent with the treatment of the jet expansion, this region of the flow is assumed to be quasi-steady.

The usual approach to modelling plume rise follows the analysis of Briggs (1984), who derived analytical expressions for plume rise assuming that the atmosphere is neutral or stable, that the "bent-over plume" assumption holds, and that the discharge is vertically upwards. Since these assumptions are not always valid to the case of sour gas releases from wells or pipelines, an alternative approach is to model the jet/plume by numerically solving the conservation equations of mass, momentum and energy as they apply to the discharged sour gas. This approach is more general than the analytical expressions for plume rise in that fewer simplifying assumptions are necessary. This approach, which has been called "integral modelling" of plumes and jets, has been employed successfully by Ooms (1972), Slawson *et al.* (1980), Schatzmann (1979), and will be used here. However, Briggs (1984) empirical correlations for limiting the final rise of momentum jets and buoyant plumes will be used in some cases.

B1.3.1 Integral Plume Rise Model

Slawson *et al.* (1980) evaluated both analytical and integral (numerical) models of plume rise as they applied to the dispersion of the Great Canadian Oil Sands Plume. They recommended an integral model for modelling the plume rise and growth of that plume. The approach adopted by this study is similar to that given by Slawson *et al.* (1980). Unlike the Slawson *et al.* approach however, this study accounts for plume "scuffing" on the ground for near horizontal releases (f_E/f_A terms) and employs different criteria for determining when the plume rise has to be terminated.

The governing conservation equations of the jet/plume may be derived from a control volume analysis of a section of the plume. The coupled set of first order ordinary differential equations for the conservation of mass, horizontal momentum, vertical momentum, energy and the concentration of a scalar (respectively) are:

$$\frac{d}{dt}(r^2 V \rho) = 2\rho_A r V V_\alpha \left(\frac{f_E}{f_A} \right) \quad (\text{B.81})$$

$$\frac{d}{dt}(r^2 V V_x \rho) = \left(\frac{f_E}{f_A} \right) [2\rho_A r U V V_\alpha + \rho_A C_{D2} r V (U - V_x) V_R] - \rho r V [\text{MAX}(0, V_x - U)]^2 C_F \frac{\sin[\pi(1 - f_E)]}{f_A} \quad (\text{B.82})$$

$$\frac{d}{dt}(r^2 V V_z \rho) = g r^2 V (\rho_A - \rho) - \rho_A C_{D2} V V_z V_R r \left(\frac{f_E}{f_A} \right) \quad (\text{B.83})$$

$$\frac{d}{dt} \left[r^2 V \rho g \left(\frac{T - T_A}{T_A} \right) \right] = \frac{\dot{q} r^2 V g}{C_{PA} \theta_A} - \frac{\rho_A r^2 V g V_z}{\theta_A} \left(\frac{d\theta_A}{dz} \right) \quad (\text{B.84})$$

$$\frac{d}{dt}(r^2 V c) = r^2 V \dot{c} \quad (\text{B.85})$$

where: t = time (s)

r = plume radius (m)

V = plume velocity (m/s)

$$= \frac{ds}{dt} = \sqrt{V_x^2 + V_z^2}$$

s = plume centreline coordinate (m)

V_x = horizontal velocity component of plume (m/s)

$$= \frac{dx}{dt}$$

x = horizontal coordinate (m)

V_z = vertical velocity component of plume (m/s)
 $= \frac{dz}{dt}$

f_E = factor to account for plume circumferential area reduction due to ground impingement ($f_E = 1$ for elevated plumes)

f_A = factor to account for plume cross-sectional area reduction due to ground impingement ($f_A = 1$ for elevated plumes)

z = vertical coordinate (m)

ρ = density of plume (kg/m^3)

ρ_A = ambient density (varies with z) (kg/m^3)

V_α = entrainment velocity, for parameterizing the amount of ambient air which is entrained into the plume (m/s)

U = ambient wind speed (varies with z) (m/s)

V_R = relative velocity between the plume and the atmosphere (m/s)
 $= \sqrt{(V_x - U)^2 + V_z^2}$

C_{D2} = drag coefficient to account for the obstruction the plume presents to the ambient flow (~ 0.5)

C_F = skin friction coefficient of plume impinging on ground ($= 0.005$)

θ = potential temperature of plume (K)

$$= T + \frac{g}{C_p} z$$

T = plume temperature (K)

C_p = specific heat at constant pressure for the plume ($\text{J}/(\text{kg K})$)

g = acceleration of gravity ($= 9.81 \text{ m/s}^2$)

C_{pA} = specific heat at constant pressure of ambient air ($\sim 997 \text{ J}/(\text{kg K})$)

θ_A = potential temperature of the atmosphere (K) (varies with z depending on stability)

$$= T_A + \frac{g}{C_{PA}} z$$

T_A = ambient temperature (varies with z) (K)

c = concentration of scalar species (e.g., H_2S) in the plume (kg/m^3)

In addition to the above variables, there are two source/sink variables which are:

$\dot{q}$ = volumetric source/sink of energy in the plume. At present $\dot{q}$ is assumed to be zero. (W/m^3)

$\dot{c}$ = volumetric source/sink of scalar species in the plume due to chemical production/depletion. At present $\dot{c}$ is assumed to be zero. (kg/s)

In order to form a closed equation set for the dependent variables ρ , V , V_x , V_z , r , θ , c , s , z and x , it remains to specify five additional independent equations:

$$\frac{d}{dt}(\rho T) = \frac{-\rho_A g V_z}{R_A} \quad (B.86)$$

$$\frac{ds}{dt} = V \quad (B.87)$$

$$\frac{dz}{dt} = V_z \quad (B.88)$$

$$\frac{dx}{dt} = V_x \quad (B.89)$$

$$\frac{dV}{dt} = \frac{V_x}{V} \frac{dV_x}{dt} + \frac{V_z}{V} \frac{dV_z}{dt} \quad (B.90)$$

where R_A = particular gas constant for air ($J/(kg \text{ K})$). The first of these additional five equations is the hydrostatic pressure law; the last four are kinematic relationships for the plume trajectory.

It should be noted that, in the derivation of the above conservation equations, "top hat" profiles (i.e., uniform in the plume cross-section) have been assumed for all the independent plume variables.

The concept behind the "scuffing" of the plume on the ground for near horizontal releases is illustrated in Figure B.3. The factor f_E appearing in the governing differential equations is an "entrainment" factor which accounts for the decrease in the circumferential surface area of the plume which is available for air entrainment when the ground "removes" the lower portion of the plume. The plume is assumed to have a circular cross-section. The f_E factor is a function of plume radius and height of the plume centreline above the ground:

$$f_E = 1 - \frac{1}{\pi} \cos^{-1} \left(1 - \frac{\delta}{r} \right) \quad (\text{B.91})$$

where:

$$\delta = \text{MAX} \left[r - \frac{z}{\cos \phi}, 0 \right] \quad (\text{B.92})$$

$$\phi = \tan^{-1} \left(\frac{V_z}{V_x} \right) \quad (\text{B.93})$$

The factor f_A appearing in the governing differential equations is a "cross-sectional area" factor which accounts for the decrease in the cross-sectional area of the plume when the ground "removes" the lower portion of the plume. The f_A factor is given by:

$$f_A = f_E + \frac{r(r - \delta)}{\pi r^2} \sin[\pi(1 - f_E)] \quad (\text{B.94})$$

Again, this factor depends on the radius of the plume and the height of the plume centreline above the ground.

In most instances, the ratio (f_E/f_A) is of primary importance for horizontal plumes in the governing differential equations. This is because the growth rate of the plume will increase if the reduction in the air entrainment is smaller than the ability of the plume to transport mass through its cross section.

The last term on the right hand side of Equation B.82 (the C_F term) accounts for the skin friction drag experienced by a plume as it scuffs across the ground. The drag is only allowed to act if the horizontal plume velocity exceeds the local wind speed. This is because the local wind speed derived from the power law wind speed profile already accounts for ground shear and it is this momentum that is entrained into the plume. The area over which the skin friction drag acts is the intersection area of the circular plume and the ground.

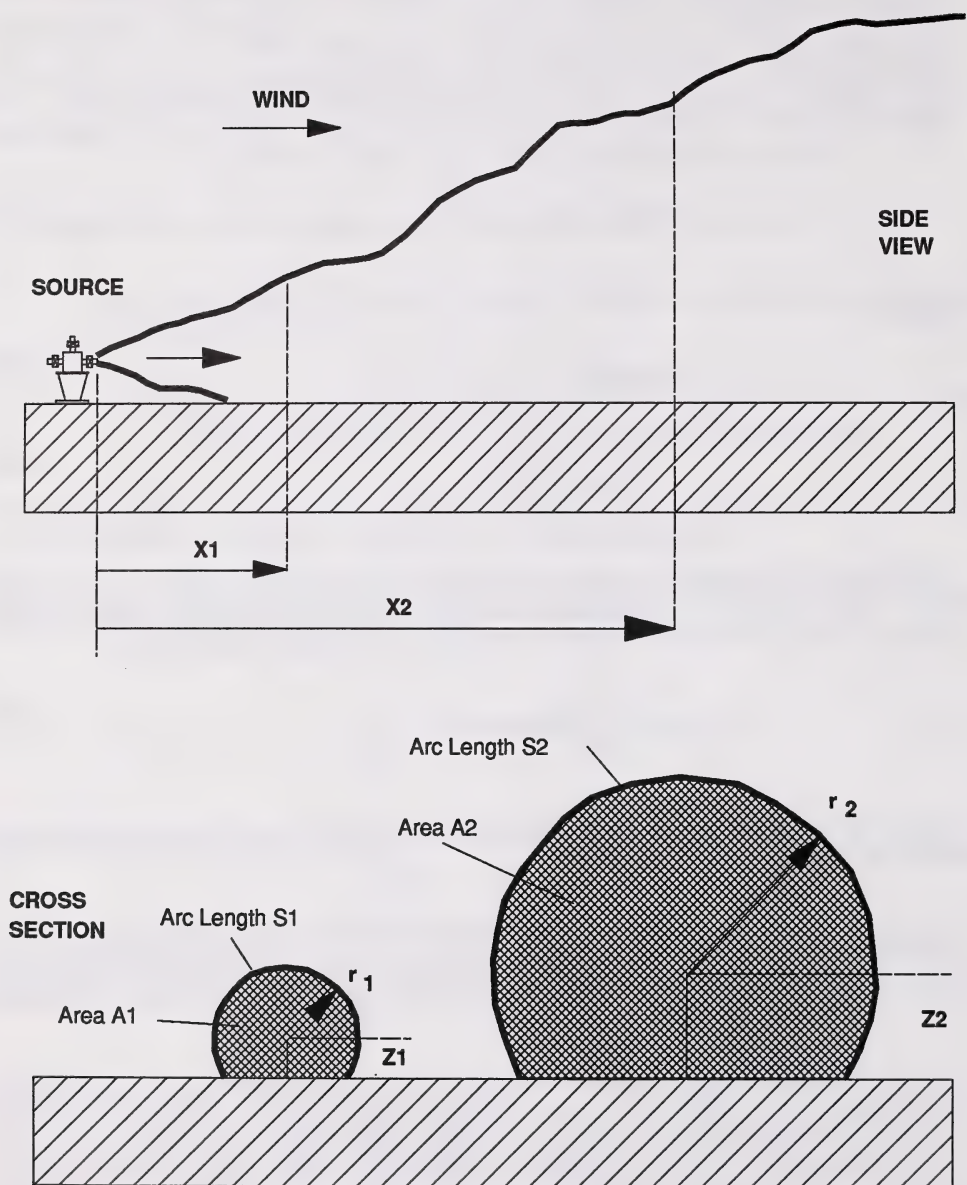


Figure B.3
Plume Scuffing for a Horizontal Plume.

The equation set for the ten independent variables is closed if the entrainment velocity V_α is specified as a function of previously defined variables. The entrainment velocity is an extremely important parameter which influences the spread of the plume. There have been many different forms for V_α suggested in the literature. A summary of various entrainment models may be found in Gebhart *et al.* (1984). The formulation used in this model has been suggested by Abraham (1971) and Ooms (1972):

$$V_\alpha = \alpha \left| V - \frac{UV_x}{V} \right| + \beta \frac{|V_x|}{V} \left| \frac{UV_z}{V} \right| \quad (\text{B.95})$$

with $\alpha \sim 0.13$ and $\beta \sim 0.58$. This form has been recommended by Slawson *et al.* (1980) and possesses the desirable property that the correct limiting forms are recovered for vertical jet entrainment near the source and bent-over plume entrainment further away.

Finally, it can be stated that the system described in this section represents a closed equation set for the variables ρ , r , V , V_x , V_z , θ , c , z , x , and s . The equations for these variables, which are coupled and non-linear, are solved by using the Livermore Solver for Ordinary Differential Equations with General Jacobian Matrices ("LSODES") (Hindmarsh, 1980), given initial values (i.e., at time $t = 0$) for the variables. The required initial values are known after the jet expansion stage of the sour gas release, as negligible time is assumed to have elapsed from the onset of the gas release. Furthermore, since transient "storage" terms have been neglected in the derivation of the conservation equations, the jet/plume is assumed to adjust instantaneously to changes in source conditions.

B1.3.2 Integral Plume Rise Termination

The numerical integration of the governing differential equations of the jet/plume yield, as part of the solution, the trajectory (z versus x) of the plume centreline. It remains to specify criteria for terminating the numerical integration once the "final rise" has occurred.

In neutral and unstable boundary layers, Slawson *et al.* (1980) suggest terminating the integral plume rise model when the plume elevation exceeds that predicted by the (standard) Briggs plume rise relations. This approach seems prudent in that the plume rise attained by the integral model is never allowed to deviate significantly from the Briggs prediction while the integral model is permitted to predict the initial dilution and downwind displacement of the plume. In this work, Briggs plume rise estimates are employed as termination criteria for the plume rise. The calculation of Briggs plume rise estimates for boundary layers of unstable, neutral or stable stability is considered in Section B1.3.3. The Briggs final plume elevation is denoted by $Z_{PF, \text{BRIGGS}}$.

In stable boundary layers, the integral plume rise model will predict a termination point when the vertical component of plume velocity is zero ($V_z = 0$). Whenever possible, this is used as the estimate of final plume elevation in a stable atmosphere, provided it is more conservative (less than) than the Briggs estimate.

In some circumstances, for neutral and unstable boundary layers, the plume rise is sufficiently slow that it is advisable to terminate the integral plume rise to save computational effort and to reduce the downwind displacement at which the calculation of ground-level concentrations may begin. The criterion:

$$\left| \frac{V_Z - 0.1V_X}{V_Z} \right| < 0.1 \quad (\text{B.96})$$

is employed as one of the integral plume termination conditions.

If the Briggs' final rise estimate $Z_{PF,BRIGGS}$ is sufficiently greater than the mixed layer height, then plume penetration will occur according to the plume penetration model described in Section B1.5.1. In this event, a better estimate of the final plume elevation is some elevation ($Z_{PF,PEN}$) less than or equal to the mixed layer height. Hence, it is more appropriate to terminate the integral plume rise model when the plume elevation exceeds the minimum of $Z_{PF,BRIGGS}$ and $Z_{PF,PEN}$.

In the stable case, termination occurs at the minimum plume elevation for which $V_Z < 0$ or at which the minimum of $Z_{PF,BRIGGS}$ and $Z_{PF,PEN}$ is exceeded; $Z_{PF,PEN}$, however, is based on the minimum of $Z_{PF,BRIGGS}$ and the elevation at which $V_Z < 0$.

If plume rise termination occurs at the " $V_Z < 0$ ", " $Z_{PF,BRIGGS}$ " or " $Z_{PF,PEN}$ " criteria, then the plume elevation is deemed to be at the maximum permissible value and the passive dispersion formulations employ a constant plume elevation at the value where the rise is terminated. If plume terminates at some earlier criterion, then the plume must be allowed to rise further to its maximum permissible elevation. To accomplish this, the plume elevation is allowed to track the following trajectory:

$$Z_P = \left[\frac{3F_M}{\beta^2 U_P^2} x_S + \frac{3}{2\beta^2} \frac{F_B x_S^2}{U_P^3} + \left(\frac{r_S}{\beta} \right)^3 \right]^{1/3} - \frac{r_S}{\beta} + Z_s \quad (\text{B.97})$$

where:

F_M = momentum flux defined in Table B.6 (m^4/s^2)

F_B = buoyancy flux defined in Table B.6 (m^4/s^3)

U_P = wind speed at plume height (m/s)

r_S = plume radius at the "S" plane in Figure B.2 (m)

β = entrainment constant = 0.58

Z_P = plume elevation (m)

x_S = virtual distance (m)

$= x - x_F + x_V$

x = downwind distance from rupture point (m)

x_F = downwind distance from rupture point when integral plume rise model is terminated (m)

x_V = distance calculated by forcing the above equation for Z_P to recover Z_F (the plume elevation when the integral plume rise model is terminated) at $x = x_F$ (m)

Z_s = elevation of "s" above the ground (m)

The above equation for Z_P is the solution to the plume equations (Equations B.81 to B.84) with the following restrictions:

- (1) Vertical discharge ($\lambda = 90^\circ$)
- (2) Neutral stability ($d\theta_A/dz = 0$)
- (3) Bent-over plume ($V_X \sim U_P$)
- (4) Constant wind speed with elevation ($U_P = \text{constant}$)
- (5) Bent-over plume entrainment ($V_\alpha = \beta |V_Z|$)
- (6) No plume drag ($C_{D2} = 0$)
- (7) Boussinesq approximation ($\rho = \rho_A$, except in buoyancy terms)

The application of Equation B.97 for Z_P continues for downwind distances as long as the maximum permissible plume elevation (given by the minimum of $Z_{PF, PEN}$ and $Z_{PF, BRIGGS}$) is not exceeded. Once the maximum elevation is attained, the plume height is considered constant at that value further downwind.

B1.3.3 Briggs' Final Plume Rise Estimates

Briggs' expressions for the final plume rise in unstable, neutral and stable atmospheres are used to arrive at the Briggs' final plume elevation $Z_{PF, BRIGGS}$.

Final Plume Rise in Unstable and Neutral Atmospheres

The Ontario Ministry of the Environment (OME) (1986) has recommended the use of Briggs' (1984) expression for the final buoyancy rise in unstable conditions:

$$(\Delta h_B)_U = 3.0Z_i \left(\frac{F_B}{W^{*2}U_P Z_i} \right)^{0.6} \quad (\text{B.98})$$

W^* = convective velocity scale from Equation 3.18 (m/s)

Z_i = mixed layer depth (m)

U_P = wind speed at plume height (m/s)

Table B.6

Buoyancy (F_B) and Momentum (F_M) Fluxes.

The buoyancy flux and momentum flux are defined as follows:

$$F_B = g V_s r_s^2 \left(\frac{\rho_A - \rho_s}{\rho_A} \right) \quad (\text{m}^4/\text{s}^3) \quad (\text{B.99})$$

$$F_M = \frac{\rho_s}{\rho_A} V_s V_{sz} r_s^2 \quad (\text{m}^4/\text{s}^2) \quad (\text{B.100})$$

where:

- ρ_A = ambient air density at ground level (kg/m^3)
- g = acceleration of gravity ($9.81 \text{ m}/\text{s}^2$)
- ρ_s = density of gas effluent at the source (kg/m^3)
- r_s = radius of effluent jet at the source (m)
- V_s = velocity of effluent jet at the source (m/s)
- V_{sz} = vertical component of V_s (m/s)
 $= V_s \sin \lambda$
- λ = angle of effluent release at source
 (with respect to the horizontal)

Note that the source parameters (ρ_s , r_s and V_s) refer to the conditions at the "S" plane for the nonignited case and the conditions at the "C" plane for the ignited case (Figure B.2).

The terminal rise due to buoyancy in a neutral boundary layer may be approximated as (Briggs, 1975):

$$(\Delta h_B)_N = \frac{1.3 F_B}{U_P U^{*2}} \left(1 + \frac{Z_s}{(\Delta h_B)_N} \right)^{2/3} \quad (\text{B.101})$$

where Z_s = initial height of the source at the "S" plane of Figure B.2 (or the "C" plane if there is ignition) (m)

The final momentum rise for both unstable and neutral conditions can be estimated from (Briggs, 1975):

$$\Delta h_M = 1.5 \left(\frac{F_M}{U_P U^*} \right)^{1/2} \quad (\text{B.102})$$

where U^* = surface friction velocity (m/s)

For very low wind speed values (as U_P approaches zero), the predicted plume rise increases rapidly (approaching infinity). The Briggs plume rise relationships for unstable and neutral conditions do not account for these near calm conditions. It is for this reason that a stable plume rise relationship applicable to near calm conditions is evaluated for low wind speed conditions:

$$\Delta h_{SC} = 5 \frac{F_B^{1/4}}{S^{3/8}} \quad (\text{B.103})$$

where the stability parameter S (s^{-2}) is given by:

$$S \equiv \frac{g}{\theta_A} \left(\frac{\partial \theta_A}{\partial Z} \right) = \frac{g}{T_A + \frac{dT_A}{dZ} Z_{SC}} \left(\frac{dT_A}{dZ} + \gamma_D \right) \quad (\text{B.104})$$

where:

- g = acceleration due to gravity (9.81 m/s^2)
- θ_A = potential temperature (K)
- $\partial \theta_A / \partial Z$ = potential temperature gradient (K/m)
- $Z_{SC} = Z_S + \Delta h_{SC}$
- dT_A / dZ = average vertical temperature gradient in the atmosphere
= -0.0065 K/m (e.g., Briggs, 1969)
- T_A = ambient temperature at Z_{REF} (K)
- γ_D = dry adiabatic lapse rate (0.0098 K/m)

The combined effect of buoyancy and momentum rise may be estimated using the "sum-of-cubes" formula recommended by Wilson (1986). Two final rises are calculated:

$$\Delta h_1 = \left[\Delta h_M^3 + \Delta h_B^3 + \left(\frac{r_s}{\beta} \right)^3 \right]^{1/3} - \frac{r_s}{\beta} \quad (\text{B.105})$$

$$\Delta h_2 = \left[\Delta h_M^3 + \Delta h_{SC}^3 + \left(\frac{r_s}{\beta} \right)^3 \right]^{1/3} - \frac{r_s}{\beta} \quad (\text{B.106})$$

where β = entrainment constant = 0.58.

Three cases need to be considered to arrive at the final Briggs plume rise value for unstable or neutral conditions (Δh):

- (1) If both plume height ($Z_s + \Delta h_1$) is greater than Z_i and ($Z_s + \Delta h_2$) is less than Z_i then $\Delta h = Z_i - Z_s$. That is, the plume height is limited by the inversion height.
- (2) If both plume heights [$(Z_s + \Delta h_1)$ and $(Z_s + \Delta h_2)$] are greater than Z_i then $\Delta h = \Delta h_2$. That is, the plume is assumed to penetrate the inversion height.
- (3) If the plume height ($Z_s + \Delta h_1$) is less than Z_i then $\Delta h = \Delta h_1$. The plume remains in the mixing layer.

where Z_s = initial height of the source at the "S" plane of Figure B.2 (or the "C" plane if there is ignition) (m) and Z_i is the depth of the mixing layer.

Finally, $Z_{PF, BRIGGS} = Z_s + \Delta h$.

Final Plume Rise in Stable Atmospheres

The final buoyancy rise in a stable atmosphere may be estimated from the following expression (Briggs, 1975):

$$(\Delta h_B)_s = 2.6 \left(\frac{F_B}{U_P S_O} \right)^{1/3} \quad (\text{B.107})$$

where S_O = the square of the Brunt-Vaisala frequency (s^{-2})

$$S_O = \frac{U^*{}^2(0.74 + 4.7Z_M/L)}{k^2 L Z_M} \quad (\text{B.108})$$

where:

- k = von Karman constant (= 0.40)
- Z_M = MAX[1, MIN(Z_s , $2L$)] (m)
- L = Monin-Obukhov length (m)

Equation B.107 is obtained by substituting the surface similarity values for θ_A and $\partial\theta_A/\partial Z$ into the definition for S (Equation B.104) (e.g., OME, 1986). According to the above definition, Z_M is not allowed to be less than 1 m or more than the minimum of Z_s or $2L$. A typical minimum value for $2L$ is 40 m.

For very low wind speed conditions (calms), estimates of the buoyancy plume rise can also be obtained from:

$$(\Delta h_B)_{SC} = 5.0 \frac{F_B^{1/4}}{S^{3/8}} \quad (\text{B.109})$$

For stable conditions, this study adopts:

$$\Delta h_B = \text{MIN}[(\Delta h_B)_S, (\Delta h_B)_{SC}] \quad (\text{B.110})$$

The final momentum rise may be approximated using:

$$\Delta h_M = 1.5 \left(\frac{F_M}{U_P S_O^{1/2}} \right)^{1/3} \quad (\text{B.111})$$

The combined effect of buoyancy and momentum rise is estimated using the "sum-of-cubes" formula recommended by Briggs (1975).

$$\Delta h = \left[\Delta h_M^3 + \Delta h_B^3 + \left(\frac{r_S}{\beta} \right)^3 \right]^{1/3} - \frac{r_S}{\beta} \quad (\text{B.112})$$

where β = entrainment constant = 0.58.

Finally, $Z_{PF, BRIGGS} = Z_S + \Delta h$.

The final stable plume elevation (Z_{PF}) is given as the minimum of the above Briggs estimate or the elevation where the integral plume rise terminates ($V_z = 0$).

B1.3.4 Accounting for Wind Speed Shear in Plume Rise

The calculation of plume rise from the integral plume model and from the Briggs plume rise relationships are dependent on the wind speed at plume height (Z_p). Plume height, of course, is not known until the plume rise is known. Therefore, the calculation of the plume rise Δh is iterative in nature. This iteration can proceed as follows:

- (1) Let $U_p = U_{REF}$ (the wind speed at anemometer height Z_{REF} , usually 10 m).
- (2) Calculate the plume rise Δh .
- (3) Calculate a new value of U_p at $Z = Z_p + \Delta h$ using the Irwin power law wind profile relationship (Equation 3.30). The wind speed U_p can never exceed the wind speed at 100 m.
- (4) Go back to (2) and recalculate Δh .
- (5) If Δh has converged to a value within 1 percent, then the iteration can be stopped. If the difference between the previous and the current estimates is greater than 1 percent, keep modifying Δh and U_p until these values converge. To reduce computational resources, no more than 15 iterations are allowed.

Normally, the height of the plume (Z_p) is greater than the reference wind speed height (Z_{REF}). Based on Equation 3.30, it follows that the wind speed at Z_p will be greater than the wind speed at Z_{REF} . The use of the larger wind speed value at Z_p in the previously discussed plume rise formulations will produce smaller plume rise values.

B1.4 Transient Release Module

Releases of toxic gas from a pipeline or a pressure vessel rupture are characterized by a time varying mass discharge rate of gas. The mass emission module used in this model for a pipeline rupture has been described in Section B1.1.2.

The steady-state plume dispersion equations (Equations B.127 and B.152) ignore diffusion in the along wind direction. For a transient release, the along wind diffusion cannot be ignored and can be accounted for by either of the following methods:

- An integrated puff model which superimposes a series of individual puffs (Section 5.4.5 from GASCON 1987 release).
- An effective mass correction which allows the use of the steady state dispersion equation (Wilson, 1979).

The first method requires considerable computer resources to superimpose the puffs. For this reason, the second method was adopted for this project.

A basic assumption in the transient module is that the rise of the effluent gas jet and plume is determined by the instantaneous mass emission rate. This means that for any downwind distance x from the rupture, the mass rate that determines the plume elevation at that distance and time is:

$$\dot{m}_E(\tau) \quad \text{where} \quad \tau = t - \frac{x}{U} \quad (\text{B.113})$$

where the transient mass rate $\dot{m}_E$ is a function of time after release as described in Section B1.1.2 and $\bar{U}$ is the mean transport wind speed of the plume. This procedure is the same as employed by Wilson (1979) where the above equation is referred to as the "frozen mass rate" (Figure B.4). The physical justification of using a frozen mass rate rather than the effective mass rate (see below) is that plume rise is related to vertical movement and along-wind diffusion will not alter the trajectory of the centre of mass to any significant extent.

The transient release module first calculates plume rise from the rupture point to the distance downwind where passive dispersion takes over the plume transport (X_F) for a number of frozen mass rates beginning with $\dot{m}_E(0)$ (the initial mass rate) and ending with MAX $[(\dot{m}_{E,S}, \dot{m}_E(99\%))]$ (the maximum of a user specified steady mass rate at large time or after 99% of the gas has been released).

A user specified number of increments between these two frozen mass rate limits are used to construct a table of frozen mass rate versus plume parameters such as:

- Plume elevation at downwind distance X_F ,
- Penetration fraction, and
- Final plume elevation.

From this table, it is thus possible to obtain plume parameters for any frozen mass rate by linear interpolation.

Two important notes need to be mentioned regarding the evaluation of frozen mass rate. First, the mean transport wind speed $\bar{U}$ is evaluated as:

$$\bar{U} = U \{ \text{MAX}[Z_{REF}, \text{MIN}(Z_{PF})] \} \quad (\text{B.114})$$

where $U(z)$ is calculated from the Irwin wind speed power law profile (Equation 3.30 from GASCON 1987 release) and $\text{MIN}(Z_{PF})$ is the minimum final plume elevation in the frozen mass rate versus plume parameter table. Second, for the lagged time $(t - x/\bar{U})$ very small, or less than zero, it is not clear what the frozen mass rate should be. In this model, the conservative assumption is made:

$$\begin{aligned} \dot{m}_E &= \dot{m}_E(0) & \text{for} & \quad t < 0 \\ &= \dot{m}_E(t) & \text{for} & \quad t \geq 0 \end{aligned} \quad (\text{B.115})$$

In order to account for along-wind diffusion of the source transient, the "effective mass flux" concept of Wilson (1981) which accounts for along wind dispersion (Figure B.4) is employed.

$$\dot{m}_{EFF}(x_1, t) = \int_{x=-\infty}^{x=\bar{U}t} \frac{\dot{m}_E(\tau)}{\sqrt{2\pi}\sigma_{x_1}} \exp\left[-\frac{(x_1 - x)^2}{2\sigma_{x_1}^2}\right] dx \quad (\text{B.116})$$

where $\dot{m}_E(\tau)$ is given by the double exponential blowdown relationship (Equation B.4) and:

$$\sigma_x = \left[0.09 \left(\frac{nx}{Z_R} \left(\frac{Z_R}{Z_V} \right)^n \right)^2 + \alpha_2 \right]^{1/2} \sigma_z \quad (\text{B.117})$$

where: σ_x = standard deviation of the transient plume in the along wind direction (x)

σ_z = standard deviation of the transient plume in the vertical direction (z)

$$Z_R = Z_p + 0.5\sigma_z$$

$$Z_V = Z_p + 0.17\sigma_z$$

Z_p = plume elevation

n = velocity profile power law exponent (Irwin model)

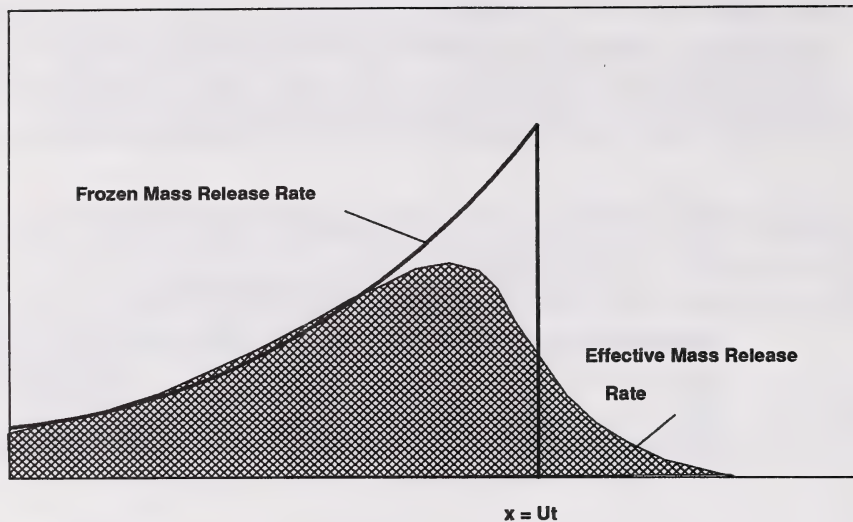
The "effective mass" $\dot{m}_{EFF}$ defined by Equation B.116 is the release rate which is used in the dispersion relationships (Equations B.127 and B.152) to estimate the ground level concentrations as a function of downwind distance. Figure B.5 illustrates that the effective mass is a function of time after the rupture and the downwind distance. A transient run involves the calculation of many effective mass rates using the method given in Table B.8.

Table B.7

Constant α_2 used to Estimate σ_x .

$\alpha_2 =$	6.0 8.0 10.0	for Unstable for Neutral for Stable
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MASS RELEASE RATE

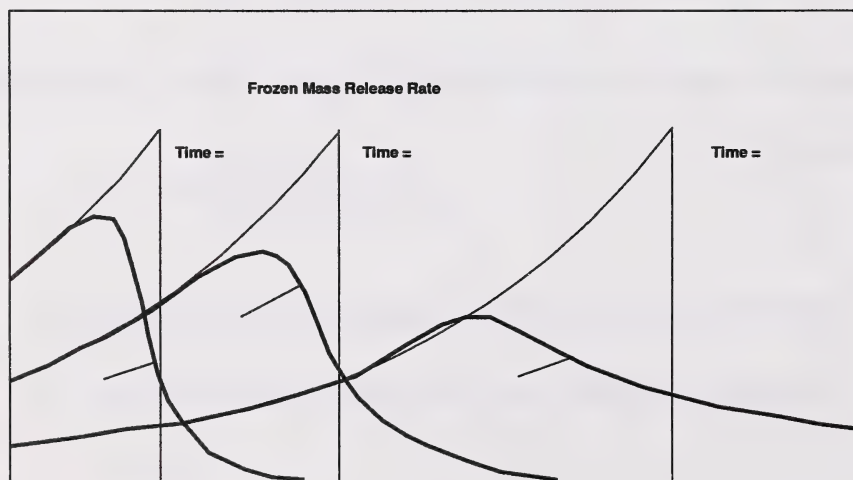


DOWNWIND DISTANCE

Figure B.4

Comparison of the "Frozen" and "Effective" Mass Release Rates.

MASS RELEASE RATE



DOWNWIND DISTANCE

Figure B.5

Frozen and Effective Mass Release Rates for Selected Times after the Rupture.

Table B.8

Analytical Expression for the Effective Mass Release Rate.

The integral expression for the effective mass release rate is computed as the sum of three terms:

$$\dot{m}_{EFF}(x_1, t) = I_1 + I_2 + I_3 \quad (\text{B.118})$$

The first and second terms account for the transient component of the mass release and the third term accounts for the steady-state component which may follow the transient portion. Specifically, the transient release terms account for each exponential term in the double exponential blowdown model (Equation B.4). The third term accounts for any steady-state release which may occur after time t_s as defined in Equation B.11. If a steady-state component is not specified, the model assumes a steady-state value equal the rate after 99% of the mass has been released.

The term I_1 represents the integration from $x = -\infty$ to $t_s \bar{U}$ of the initial rapid decay transient (first term in Equation B.4):

$$[\text{EQUATION}] \quad (\text{B.119})$$

The term I_2 also represents the integration from $x = -\infty$ to $t_s \bar{U}$ of the final slow decay transient (second term in Equation B.4):

$$[\text{EQUATION}] \quad (\text{B.120})$$

$$I_3 = \begin{matrix} 0 & t < t_s \\ \dot{m}_{E,S} & t \geq t_s \end{matrix} \quad (\text{B.121})$$

B1.5 Passive Dispersion Module

During the jet expansion stage of a sour gas release, the behavior of the jet itself determines the initial trajectory and dilution of the plume; the turbulent behavior of the atmosphere is of secondary importance during this stage. At the completion of the jet dominated stage, the mean motion and turbulence of the atmosphere begin to dominate plume dispersion processes.

The ability of the atmosphere to disperse a plume is dependent on the level of turbulence in the atmosphere and on the presence of physical boundaries which restrict plume spread. Typical boundaries include the top of the mixed layer (upper boundary) and the ground (lower boundary). The relative location of the plume (after reaching final rise) with respect to these two boundaries is important in determining the dilution of the plume. Figure B.6 illustrates three possible plume-boundary combinations:

- The plume is located very near or above the top of the mixed layer. The plume rise may, in certain conditions, be sufficient to allow the plume to penetrate the mixed layer. When this occurs, the downwind concentrations of plume gases will be reduced.
- The plume is elevated. This condition is most frequently assumed in the prediction of plume concentrations resulting from industrial stacks. The plume is usually assumed to have a Gaussian shape in both the vertical and the lateral directions.
- The plume is located near the surface. Due to limited plume rise, the plume remains sufficiently near the surface that the presence of the ground results in a non-Gaussian shape in the vertical direction.

The following discussion considers these three plume-boundary condition combinations with respect to unstable, neutral and stable atmospheres in the prediction of ground level plume concentrations.

B1.5.1 Plume Penetration of the Mixed Layer

Neutral and Stable Conditions

From the final plume rise estimates, it is possible to predict if the jet/plume will interact with the top of the mixed layer. If some of the plume penetrates the mixed layer then downwind ground-level concentrations of toxic gas will be proportionally reduced. The plume penetration model represented by the following relationships is applied to both neutral and stable boundary layers.

If f represents the fraction of the plume remaining below the mixed layer height Z_i , then OME (1986) suggests:

$$\begin{aligned} f &= 1 & \text{if } Z_i > Z_s + 1.5 \Delta h \\ f &= (Z_i - Z_s)/\Delta h - 0.5 & \text{if } Z_s + 0.5 \Delta h < Z_i < Z_s + 1.5 \Delta h \end{aligned} \quad (\text{B.122})$$

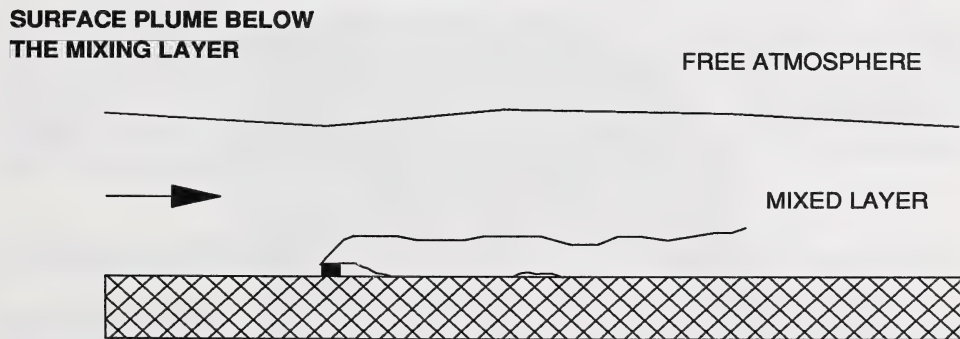
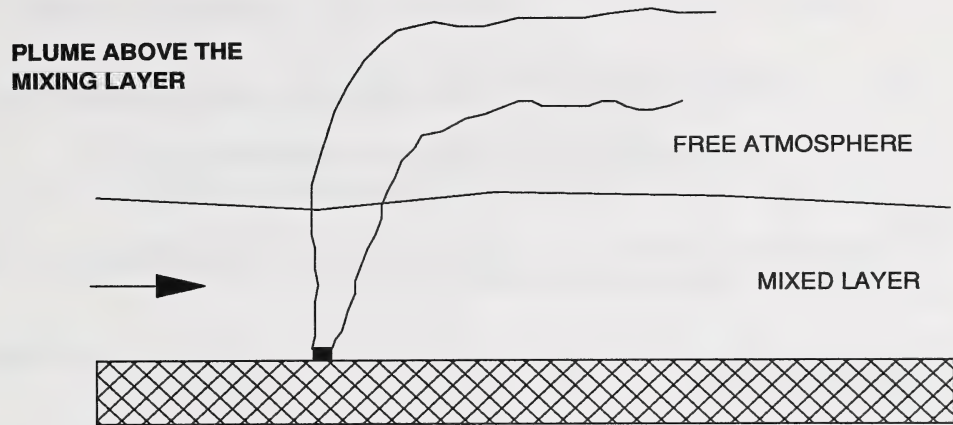


Figure B.6
Three Possible Plume-Boundary Conditions.

$$f = f_{MIN} \quad \text{if } Z_i < Z_s + 0.5 \Delta h$$

where:

- Z_i = mixed layer height (m)
- Z_s = height of the "S" plane in the jet expansion region (or the "C" plane, if there is ignition) (m)
- Δh = final plume rise estimate, as in Section B1.3 (m)
- f = plume fraction remaining inside the mixed layer.

The value for f is not allowed to be less than f_{MIN} as discussed in the next subsections. Figure B.7 illustrates the above relationships schematically.

If plume penetration is predicted to occur ($f < 1$), then the final elevation of the plume is given as (OME, 1986):

$$Z_{PF,PEN} = \text{MIN} \left[\frac{(Z_i + Z_s)}{2} + \frac{\Delta h}{4}, Z_i \right] \quad (\text{B.123})$$

where $Z_{PF,PEN}$ = the final plume elevation from the penetration model (m).

When the plume reaches its final rise elevation (given by either the above relationship or similar relationships given in the Plume Rise Module Section) the fraction f is used to modify the mass flow $\dot{m}_E$ appearing in the passive dispersion parameterizations.

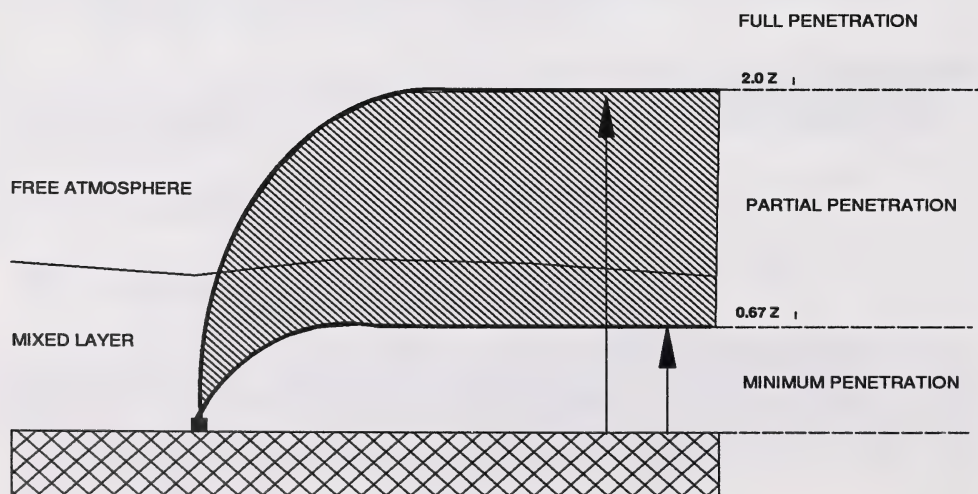


Figure B.7

Plume Penetration Factor f as a Function of Plume Height and Mixing Height for Neutral and Stable Conditions.

Unstable Conditions

The Manins (1979) plume penetration model is used for unstable conditions:

$$f = \text{fraction of the plume remaining within the mixing layer}$$
$$= 0.08 \left(1 + \frac{1}{P} \right) - P \quad (\text{B.124})$$

where:

$$P = \frac{F_B}{U_P b_I (Z_i - Z_S)^2} \quad (\text{B.125})$$

U_P = wind speed at plume height (m/s)

F_B = buoyancy flux of the plume (m^4/s^3)

b_I = strength of the inversion (m/s^2)
= $g (\Delta\theta_I)/\theta_A$

$\Delta\theta_I$ = change in potential temperature across the depth of the inversion (K)
= 10 K (Ley, 1986)

Z_i = mixed layer height (m)

Z_S = source height (m)

θ_A = potential temperature at plume height (K)

The value for f is not allowed to be less than f_{MIN} as discussed in the next subsection.

While this model is simple, it is based on buoyancy flux rather than plume rise (as is the penetration model for neutral and stable atmospheres). It is therefore difficult to incorporate the effects of momentum flux in the plume penetration model. By only considering F_B , it is felt that plume penetration for unstable conditions will err on the conservative side. It is anticipated that that plume penetration will be an important factor for ignited release cases where the buoyancy rise will clearly dominate the momentum rise.

Minimum Penetration

As the plume from a surface based release rises through the mixing layer, portions of the plume edge are expected to be entrained into the mixing layer due to atmospheric and plume generated turbulence which would preclude complete penetration. That is, f should never equal zero. For this reason a minimum value for f is estimated from:

$$f_{MIN} = f + f_{EDGE}(1 - f) \quad (\text{B.126})$$

where: f_{MIN} = Minimum value of f used in Equations B.127 and B.152.
 f = Predicted values of f from Equations B.122 and B.124.
 f_{EDGE} = Entrainment value to define f_{MIN} .
= 0.05

The value of f_{EDGE} is expected to be a function of atmospheric stability and the time the plume spends in the mixing layer. Larger levels of turbulence and longer times in the mixing layer are expected to contribute to producing a larger value of f_{EDGE} . In the absence of observations for f_{EDGE} , a single value of 0.05 was assumed.

B1.5.2 Elevated Releases

Elevated plume releases assume the frequently used Gaussian plume model (e.g. Turner, 1970). This model assumes that the distribution of plume material in the vertical and crosswind directions have a Gaussian or normal distribution. The ground level concentration is given by:

$$\chi(x, y, z) = \frac{\dot{m}_p}{2\pi U_p \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left\{ \exp\left[-\frac{(z - Z_p)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z + Z_p)^2}{2\sigma_z^2}\right] \right\} \quad (\text{B.127})$$

where: $\chi(x, y, z)$ = concentration of a given plume component (H_2S or SO_2) at position (x, y, z) (kg/m^3)
 x = downwind distance from the rupture point (m)
 y = crosswind distance (m)
 z = height above ground level (m)
 f = fraction of the plume remaining below the mixed layer height
 $\dot{m}_p$ = mass flow of the given plume component (H_2S or SO_2) in the release (kg/s)
 U_p = wind speed at plume height (m/s). The wind speed at plume height is used since an average plume element spends most of its time at this height.
 σ_y = standard deviation of the plume in the crosswind direction (m)
 σ_z = standard deviation of the plume in the vertical direction (m)
 Z_p = height of the plume above ground level (m).

The criteria for determining whether a plume is classified as an elevated release (as opposed to a surface release) is stability dependent. The criteria for an elevated release are given as:

- Unstable $Z_{PF} > |L|$
 - Neutral $Z_{PF} > 0$
 - Stable $Z_{PF} > L/50$
- (B.128)

where: Z_{PF} = final height of the plume above ground level or in the case of partial plume penetration, the height of the remaining portion of the plume in the mixed layer (m)
 L = Monin-Obukhov length (m).

The methods for estimating the plume standard deviations (σ_Y and σ_Z) are also stability dependent and are given in the following sections.

Unstable Conditions

For unstable conditions, the Weil and Brower (1984) model is used to estimate plume standard deviations for elevated releases:

$$\sigma_Y = \left[0.0064 + 0.3136 \left(\frac{W^*}{U_{REF}} \right)^2 \right]^{1/2} X_{SY} f_{CY} \quad (B.129)$$

$$\sigma_Z = \left[0.0036 + 0.3136 \left(\frac{W^*}{U_{REF}} \right)^2 \right]^{1/2} X_{SZ} f_{CZ} \quad (B.130)$$

where:

- X_{SY} = distance from a virtual y-source (m)
- X_{SZ} = distance from a virtual z-source (m)
- f_{CY} = dimensionless correction factor to force the Weil and Brower σ_Y values to equal the Briggs (1974) σ_Y values at large distances
- f_{CZ} = dimensionless correction factor to force the Weil and Brower σ_Z values to equal the Briggs (1974) σ_Z values at large distances
- W^* = convective velocity scale (Equation 3.18 from GASCON 1987 release)

The virtual source distances account for the initial spread of the plume calculated from the integral plume rise module. The virtual source distances (X_{SY} and X_{SZ}) are estimated from the relationships given in Table B.9.

The virtual distances X_{VY} and X_{VZ} are given by forcing the plume radius R_F at the distance X_F to equal twice the plume standard deviations:

$$X_{VY} = \frac{R_F}{2} \left[0.0064 + 0.3136 \left(\frac{W^*}{U_{REF}} \right)^2 \right]^{-1/2} \frac{1}{f_{CY}} \quad (B.131)$$

$$X_{VZ} = \frac{R_F}{2} \left[0.0036 + 0.3136 \left(\frac{W^*}{U_{REF}} \right)^2 \right]^{-1/2} \frac{1}{f_{CZ}} \quad (B.132)$$

Table B.9

Virtual Source Concept for Elevated Plumes.

The virtual source distances are defined by:

$$X_{SY} = x - X_F + X_{VY} \quad (\text{B.133})$$

$$X_{SZ} = x - X_F + X_{VZ} \quad (\text{B.134})$$

where:

- x = downwind distance from release point to where the ambient concentration is to be calculated (m)
- X_F = downwind distance from release point to where the integral plume rise has terminated (m)
- X_{VZ} = virtual distance to account for the spread of the plume in the vertical direction (m)
- X_{VY} = virtual distance to account for the spread of the plume in the crosswind direction (m)

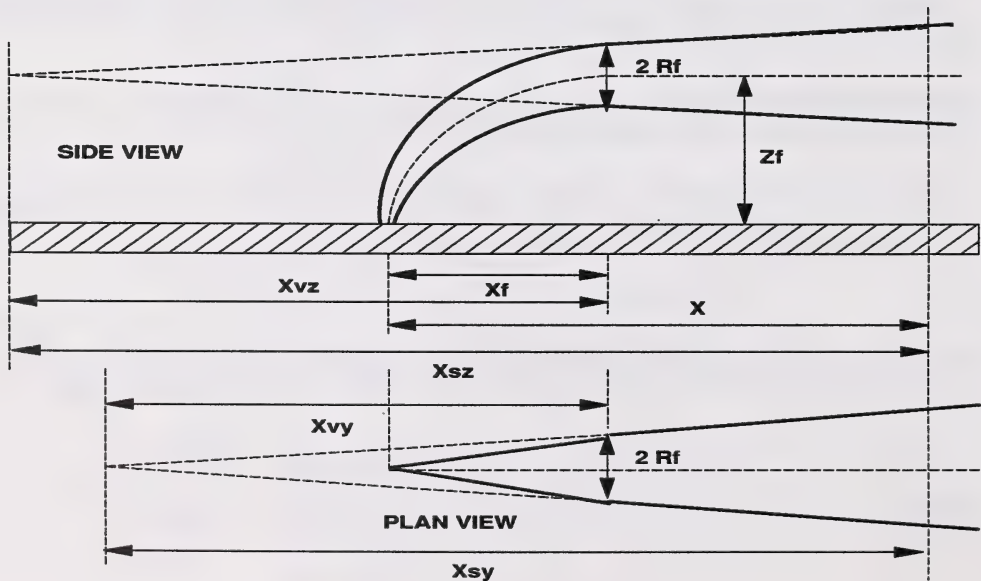


Figure B.8

Virtual Source Concept for Elevated Plumes.

The correction factors f_{CY} and f_{CZ} are required since the Weil and Brower σ_Y and σ_Z values are only applicable near the source. These factors ensure that the Weil and Brower values (Equations B.129 and B.130) converge to the σ_Y and σ_Z values given by Briggs (1974) for large downwind distances. The Briggs values are applicable to open country conditions for downwind distances less than 10 km. The correction factors were empirically determined to be:

$$f_{CY} = \frac{1}{1 + \frac{x}{30,000}} \quad (\text{B.135})$$

$$f_{CZ} = \left\{ \left[\left(\frac{U_{REF}}{6W^*} \right)^{0.12} x^{(0.04 - 0.011U_{REF}/W^*)} \right]^2 + \left[\frac{300U_{REF}^2}{(13.9W^*)^2 (400 + x^{0.75})} \right]^2 \right\}^{1/2} \quad (\text{B.136})$$

Neutral Conditions

For neutral conditions, the Briggs' (1974) model corresponding to open country conditions for downwind distances less than 10 km is used to estimate plume standard deviations for elevated releases:

$$\sigma_Y = \frac{0.08X_{SY}}{(1 + 0.0001X_{SY})^{1/2}} \quad (\text{B.137})$$

$$\sigma_Z = \frac{0.06X_{SZ}}{(1 + 0.0015X_{SZ})^{1/2}} \quad (\text{B.138})$$

where: X_{SY} = distance from a virtual y-source (m)
 X_{SZ} = distance from a virtual z-source (m)

The virtual source distances account for the initial spread of the plume calculated from the integral plume rise module. The virtual source distances (X_{SY} and X_{SZ}) are also estimated from the relationships given in Table B.9.

The virtual distances X_{VY} and X_{VZ} are given by forcing the plume radius R_F at the distance X_F to equal twice the plume standard deviations and can be obtained from the solution to the following equations:

$$\frac{R_F}{2} = \frac{0.08X_{VY}}{(1 + 0.0001X_{VY})^{1/2}} \quad (\text{B.139})$$

$$\frac{R_F}{2} = \frac{0.06X_{VZ}}{(1 + 0.0015X_{VZ})^{1/2}} \quad (\text{B.140})$$

Stable Conditions

For stable conditions, the following model is used to estimate plume standard deviations for elevated releases:

$$\sigma_Y = \frac{\sigma_v X_{SY}}{U_{REF}} f_Y(X_{SY}) \quad (\text{B.141})$$

$$\sigma_Z = \frac{\sigma_w X_{SZ}}{U_{REF}} f_Z(X_{SZ}) \quad (\text{B.142})$$

where:

X_{SY} = distance from a virtual y-source (m)

X_{SZ} = distance from a virtual z-source (m)

σ_v = standard deviation of the crosswind speed fluctuations (radian)

σ_w = standard deviations of the vertical wind speed fluctuations (radian)

U_{REF} = wind speed at reference (anemometer) height (m/s)

$f_Y(x)$ = dimensionless function which relates crosswind velocity fluctuations to crosswind plume spread

$f_Z(x)$ = dimensionless function which relates vertical wind velocity fluctuations to vertical plume spread

The virtual source distances account for the initial spread of the plume calculated from the integral plume rise module. The virtual source distances (X_{SY} and X_{SZ}) are estimated from the relationships given in Table B.9.

The virtual distances X_{VY} and X_{VZ} for stable conditions are given by forcing the plume radius R_F at the distance X_F to equal twice the plume standard deviation and can be obtained from the solution to the following equations:

$$\frac{R_F}{2} = \frac{\sigma_v X_{VY}}{U_{REF}} f_Y(X_{VY}) \quad (\text{B.143})$$

$$\frac{R_F}{2} = \frac{\sigma_w X_{VZ}}{U_{REF}} f_Z(X_{VZ}) \quad (\text{B.144})$$

Based on Nieuwstadt (1984) and Weil (1985), the standard deviation of the vertical velocity fluctuation can be estimated from:

$$\sigma_w = 1.3U^* \left(1 - \frac{Z_P}{Z_i} \right)^{3/4} \quad (\text{B.145})$$

Based on the Hanna (1981) and Pasquill and Smith (1983) interpretations of the 1973 Minnesota Experiment turbulence data (Kaimal *et al.*, 1978) and Weil (1985), the standard deviation of the crosswind velocity fluctuation can be estimated from:

$$\sigma_v = 1.94U^* \left(1 - \frac{Z_p}{Z_i}\right)^{3/4} \quad (\text{B.146})$$

The "3/4" power is an average of the "1" power recommended by Hanna (1981) and the "1/2" power recommended by Pasquill and Smith (1983). The "3/4" value is also consistent with formulation used to estimate σ_w .

The Gaussian plume model assumes that σ_v and σ_w are constant with height whereas Equations B.145 and B.146 assume that σ_v and σ_w vary with height. For example, the value for σ_w varies from $1.3 U^*$ at $z = 0$ to zero at $z = Z_i$. Similarly, σ_v varies from $1.94 U^*$ at $z = 0$ to zero at $z = Z_i$. Wilson (1987) started with the above formulations for the σ_v and σ_w profiles and recommended that weighted average values of σ_v and σ_w between height $z = 0$ and $z = Z_p$ for use in a Gaussian plume model be estimated from:

$$\sigma_v = \frac{0.485U^* \left(\frac{Z_p}{Z_i}\right)}{1 - \left[1 - \frac{Z_p}{Z_i}\right]^{1/4}} \quad (\text{B.147})$$

$$\sigma_w = \frac{0.325U^* \left(\frac{Z_p}{Z_i}\right)}{1 - \left[1 - \frac{Z_p}{Z_i}\right]^{1/4}} \quad (\text{B.148})$$

The above effective values for σ_v and σ_w account for the trajectory of an individual plume element which spends a larger fraction of the time near the plume centreline.

The dimensionless functions $f_Y(x)$ and $f_Z(x)$ are taken from Pasquill (1976) and Irwin (1983):

$$f_Y(x) = \frac{1}{1 + \left(\frac{x}{2500}\right)^{1/2}} \quad \text{for} \quad x \leq 10^4 \text{ m} \quad (\text{B.149})$$

$$f_Y(x) = \frac{33}{x^{1/2}} \quad \text{for} \quad x > 10^4 \text{ m} \quad (\text{B.150})$$

$$f_Z(x) = \frac{1}{1 + 0.9 \left(\frac{x}{50U_p}\right)^{1/2}} \quad \text{for} \quad x \leq 10^4 \text{ m} \quad (\text{B.151})$$

The function $f_Y(x)$ has the property of equalling one at $x = 0$ m and decreasing to 0.33 at $x = 10^4$ m. Similarly $f_Z(x)$ also equals one at $x = 0$ m and decreases to 0.10 at $x = 10^4$ m (with $U_p = 2$ m/s). In the application of the above dimensionless functions, X_{SY} is substituted for x in the estimation of $f_Y(x)$ and X_{SZ} is substituted for x in the estimation of $f_Z(x)$.

Low Wind Speed Stable Conditions

Due to the importance of low wind speed, stable conditions in modelling the dispersion of uncontrolled sour gas releases (Sections 5.2.2 and 5.2.4 from GASCON 1987 release), some further discussion on the subject is warranted.

Under these conditions, plume meandering can increase the horizontal plume spread values (σ_Y). The larger the averaging period, the larger the σ_Y values can become. For the estimation of three minute average concentrations, the meandering effect is expected to be minimal. The estimation of hourly average concentrations using models which ignore plume meander has led to overpredictions ranging from a factor of 10 for flat terrain to a factor of 100 for rolling forested terrain (Draxler, 1984; Van der Hoven, 1976).

The estimation of σ_Y from Equation B.141 does not account for plume meander. Therefore, caution should be exercised in the interpretation of the low wind speed values in stable atmospheres, especially for averaging periods larger than 3 minutes.

B1.5.3 Surface Releases

For near surface plume releases, van Ulden's (1978) model is used to estimate crosswind integrated (CWI) ground level plume concentrations. The distribution of plume material in the crosswind direction is assumed to have a Gaussian or normal distribution. The vertical spread of the plume is assumed to follow the exponential form given by Horst (1979). With these assumptions, the ambient concentration is given by:

$$\chi(x, y, z) = \frac{0.73 f \dot{m}_p}{\sqrt{2\pi} \bar{U} \sigma_y \bar{Z}} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left[-\left(\frac{z}{1.52\bar{Z}}\right)^2\right] \quad (\text{B.152})$$

where: $\chi(x, y, z)$ = concentration of a given plume component (H_2S or SO_2) at position (x, y, z) (kg/m^3)

x = downwind distance from the rupture point (m)

y = crosswind distance (m)

z = height above ground level (m)

f = fraction of the plume remaining below the mixed layer height

$\dot{m}_p$ = mass flow of the given plume component (H_2S or SO_2) in the release (kg/s)

$\bar{U}$ = mean transport wind speed for the plume (m/s)

$\bar{Z}$ = mean height to which plume has dispersed (m)

σ_y = standard deviation of the plume in the crosswind direction (m)

Ground-level concentrations for distances less than $5X_{yy}$ from the source should be used with caution. This is because Equation B.152 implicitly assumes a ground release and accounts for nonzero releases by assuming a virtual source correction factor (Equations B.162, B.169 and B.177 for unstable, neutral and stable conditions, respectively). The virtual source correction can produce the most uncertainty near the source for unstable conditions. A typical value for $5X_{yy}$ under these conditions is 500 m.

The criteria for determining whether a plume is classified as a surface release (as opposed to an elevated release) is stability dependent. These criteria are given as:

- Unstable $Z_{PF} < |L|$
- Neutral $Z_{PF} = 0$
- Stable $Z_{PF} < L/50$

where: Z_{PF} = final height of the plume above ground level (m)

L = Monin-Obukhov length (m).

For stable conditions, the maximum allowable value for L is 500 m (Section 3.1.5 from Gascon 1987 release). Therefore, under stable conditions, surface releases will not be assumed if Z_{PF} is greater than 10 m. For unstable conditions, $|L|$ can typically vary between 10 and 100 m. Therefore, under unstable conditions, typical Z_{PF} values will be less than 10 to 100 m before surface release conditions are assumed.

The methods for estimating the plume standard deviation (σ_y), the mean transport wind speed ($\bar{U}$) and the mean plume height ($\bar{Z}$) are also stability dependent and are given in the following sections.

Unstable Conditions

For surface releases under unstable conditions:

$$\sigma_y = \frac{0.6Z_i X_{SY}^*}{(1 + 0.7X_{SY}^*)^{1/2}} f_y(X_{SY}) \quad (\text{B.153})$$

$$\begin{aligned} \bar{Z} &= 0.812Z_i X_{SZ}^{*3/2} & \text{if } \bar{Z} < Z_i \\ &= Z_i & \text{if } \bar{Z} \geq Z_i \end{aligned} \quad (\text{B.154})$$

$$\bar{U} = U_p \quad (\text{B.155})$$

where:

$$\begin{aligned} X_{SY}^* &= \text{non-dimensional distance from a virtual y-source} \\ &= \frac{X_{SY} W^*}{U_{REF} Z_i} \end{aligned}$$

$$\begin{aligned} X_{SZ}^* &= \text{non-dimensional distance from a virtual z-source} \\ &= \frac{X_{SZ} W^*}{U_{REF} Z_i} \end{aligned}$$

Z_i = height of the mixed layer (m)

W^* = convective velocity scale (m/s)

X_{SY} = distance from a virtual y-source (m)

X_{SZ} = distance from a virtual z-source (m)

U_p = wind speed at plume height (m/s)

$f_y(x)$ = dimensionless function which relates crosswind velocity fluctuations to crosswind plume spread.

$$f_y(x) = \frac{1}{1 + \frac{x}{30000}}$$

The virtual source distance accounts for the initial spread of the plume calculated from the integral plume rise module and for non-zero source heights. The virtual source distance (X_{SY} and X_{SZ}) is estimated from the relationships given in Table B.10.

Table B.10

Virtual Source Concept for Surface Plumes.

The virtual source distances are defined by:

$$X_{SY} = x - X_F + X_{VY} \quad (\text{B.156})$$

$$X_{SZ} = x - X_F + X_{VZ} + X_O \quad (\text{B.157})$$

where:

- x = downwind distance from release point to where the ambient concentration is to be calculated (m)
- X_F = downwind distance from release point to where the integral plume rise has terminated (m)
- X_{VY} = virtual distance to account for the spread of the plume in the vertical direction (m)
- X_{VZ} = virtual distance to account for the spread of the plume in the crosswind direction (m) $X_{VZ} = X_{VY}$
- X_O = virtual distance to account for a non-zero ground release in the estimation of vertical exponential profile (m)

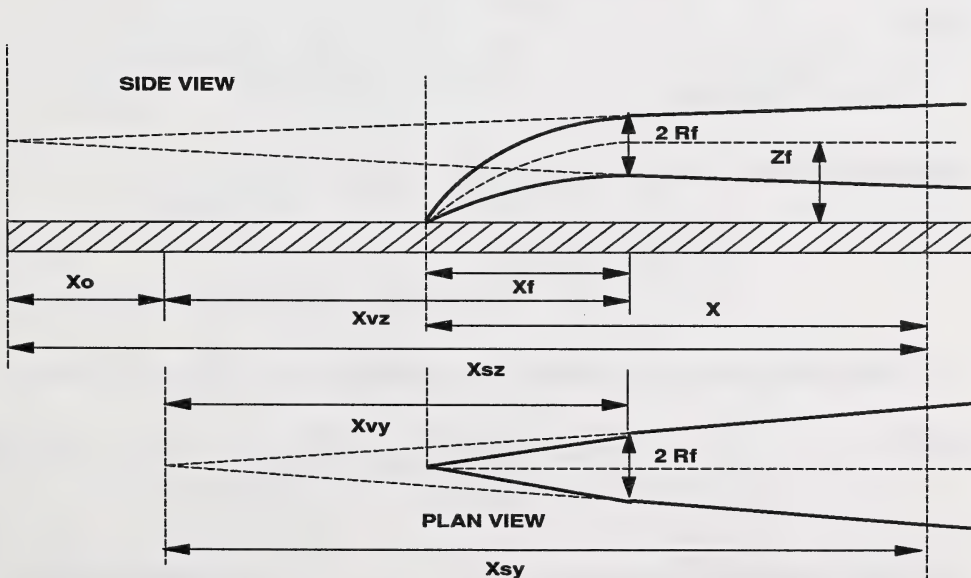


Figure B.9

Virtual Source Concept for Surface Plumes.

The virtual distance X_{vy} for unstable conditions is given by forcing the plume radius R_F at the distance X_F to equal twice the plume standard deviation and may be obtained by solving:

$$\frac{R_F}{2} = \frac{0.6Z_i X_{vy}^*}{(1 + 0.7X_{vy}^*)^{1/2}} \quad (\text{B.158})$$

with:

$$X_{vy}^* = \frac{X_{vy} W^*}{U_{REF} Z_i} \quad (\text{B.159})$$

The virtual distance X_o for unstable conditions is given by solving:

$$X_o^* = \left(\frac{Z_F}{0.812Z_i} \right)^{2/3} \quad \text{if} \quad Z_F < Z_i \quad (\text{B.160})$$

$$X_o^* = \left(\frac{1}{0.812} \right)^{2/3} = 1.149 \quad \text{if} \quad Z_F \geq Z_i \quad (\text{B.161})$$

with:

$$X_o^* = \frac{X_o W^*}{U_{REF} Z_i} \quad (\text{B.162})$$

Neutral Conditions

For surface releases under neutral conditions:

$$\sigma_Y = \frac{\sigma_v X_{SY}}{U_{REF}} f_Y(X_{SY}) \quad (\text{B.163})$$

The mean plume height ($\bar{Z}$) is given by the solution of:

$$X_{SZ} = \frac{0.74\bar{Z}}{k^2} \ln \left(\frac{0.6\bar{Z}}{Z_o} \right) \quad (\text{B.164})$$

The mean wind speed ($\bar{U}$) is given by:

$$\bar{U} = \frac{U^*}{k} \ln \left(\frac{0.6\bar{Z}}{Z_o} \right) \quad (\text{B.165})$$

where:

- X_{SY} = distance from a virtual y-source (m)
- X_{SZ} = distance from a virtual z-source (m)
- σ_V = standard deviation of the crosswind speed fluctuations (radian)
- U_{REF} = wind speed at reference (anemometer) height (m/s)
- $f_Y(x)$ = dimensionless function which relates crosswind velocity fluctuations to crosswind plume spread
- k = von Karman constant (~ 0.4)
- Z_o = surface roughness length (m)

The virtual source distances account for the initial spread of the plume calculated from the integral plume rise module and the non-zero release point. The virtual source distances (X_{SY} and X_{SZ}) are estimated from the relationships given in Table B.10.

The virtual distance X_{VY} for neutral conditions is given by forcing the plume radius R_F at the distance X_F to equal twice the plume standard deviation and can be obtained from the solution to the following equation:

$$\frac{R_F}{2} = \frac{1.3U^*X_{VY}}{U_P} f_Y(X_{VY}) \quad (B.166)$$

The dimensionless function $f_Y(x)$ is based on Pasquill (1976) and Irwin (1979):

$$f_Y(x) = \frac{1}{1 + \left(\frac{x}{2500}\right)^{1/2}} \quad \text{for} \quad x \leq 10^4 \text{ m} \quad (B.167)$$

$$f_Y(x) = \frac{33}{x^{1/2}} \quad \text{for} \quad x > 10^4 \text{ m} \quad (B.168)$$

In the application of $f_Y(x)$, X_{VY} is substituted for x .

The virtual distance X_O for neutral conditions is given by:

$$X_O = \frac{0.74Z_F}{k^2} \ln \left(\frac{0.6Z_F}{Z_o} \right) \quad (B.169)$$

Stable Conditions

For stable conditions, the following model is used to estimate plume standard deviation for surface releases:

$$\sigma_Y = \frac{\sigma_v X_{SY}}{U_{REF}} f_Y(X_{SY}) \quad (B.170)$$

The mean plume height is obtained by solving the implicit equation:

$$X_{SZ} = \frac{0.74\bar{Z}}{k^2} \left\{ \ln \left(\frac{0.6\bar{Z}}{Z_o} \right) + 4.9 \frac{\bar{Z}}{L} \left[1 + \frac{4.9\bar{Z}}{L} \right] + \frac{1.2\bar{Z}}{L} \right\} \quad (B.171)$$

The mean wind speed is given by:

$$\bar{U} = \frac{U^*}{k} \left[\ln \left(\frac{0.6\bar{Z}}{Z_o} \right) + 4.7 \frac{\bar{Z}}{L} \right] \quad (B.172)$$

where:

X_{SY} = distance from a virtual y-source (m)

X_{SZ} = distance from a virtual z-source (m)

σ_v = standard deviation of the crosswind speed fluctuations (radian)

σ_w = standard deviations of the vertical wind speed fluctuations (radian)

U_{REF} = wind speed at reference (anemometer) height (m/s)

$f_Y(x)$ = dimensionless function which relates crosswind velocity fluctuations to crosswind plume spread

The virtual source distances account for the initial spread of the plume calculated from the integral plume rise module and the non-zero release point. The virtual source distances (X_{SY} and X_{SZ}) are estimated from the relationships given in Table B.10.

The virtual distance X_{VY} for stable conditions is given by forcing the plume radius R_F at the distance X_F to equal twice the plume standard deviation and can be obtained from the solution to the following equation:

$$\frac{R_F}{2} = \frac{\sigma_v X_{VY}}{U_{REF}} f_Y(X_{VY}) \quad (B.173)$$

The standard deviation of the crosswind velocity fluctuation is estimated from the same relationship used for elevated plumes in stable atmospheres. This relationship was based on the Wilson (1987) modification to the σ_v formulations proposed by the Hanna (1981) and Pasquill and Smith (1983) interpretations of the 1973 Minnesota Experiment turbulence data (Kaimal *et al.*, 1978) and Weil (1985):

$$\sigma_v = \frac{0.485 U^* \left(\frac{Z_p}{Z_i} \right)}{1 - \left[1 - \frac{Z_p}{Z_i} \right]^{1/4}} \quad (B.174)$$

The dimensionless function $f_Y(x)$ is based on Pasquill (1976) and Irwin (1979):

$$f_Y(x) = \frac{1}{1 + \left(\frac{x}{2500}\right)^{1/2}} \quad \text{for} \quad x \leq 10^4 \text{ m} \quad (\text{B.175})$$

$$f_Y(x) = \frac{33}{x^{1/2}} \quad \text{for} \quad x > 10^4 \text{ m} \quad (\text{B.176})$$

The function $f_Y(x)$ has the property of equalling one at $x = 0$ m and decreasing to 0.33 at $x = 10^4$ m. In the application of $f_Y(x)$, X_{SY} is substituted for x .

The virtual distance X_O is given by:

$$X_O = \frac{0.74Z_F}{k^2} \left\{ \ln \left(\frac{0.6Z_F}{Z_O} \right) + 4.9 \frac{Z_F}{L} \right\} \left[1 + \frac{4.9Z_F}{L} + \frac{1.2Z_F}{L} \right] \quad (\text{B.177})$$

B1.5.4 The Correction of Concentrations for Averaging Time

The horizontal plume spread values used in this work are interpreted to be representative of 30 minute averaging times. Often, concentration limits are specified for another averaging time, requiring a conversion of the horizontal plume spreads from the 30 minute value to the specified value. The formulation used in this work for steady-state conditions is (e.g., Pasquill and Smith, 1983):

$$\frac{\sigma_{Y2}}{\sigma_{Y1}} = \left(\frac{t_2}{t_1} \right)^{q_T} \quad (\text{B.178})$$

where:

- σ_{Y1} = horizontal plume spread for averaging time t_1 (m)
- t_1 = averaging time (s)
- σ_{Y2} = horizontal plume spread for averaging time t_2 (m)
- t_2 = averaging time (s)
- q_T = an exponent which depends on atmospheric stability

There is some variation in the literature as to the appropriate values to use for q_T . The values used in this work are as follows:

- Unstable 0.40
- Neutral 0.30
- Stable 0.15

These values are similar to values of q_T given by the Texas Air Control Board (1979) and the International Atomic Energy Agency (1980). No averaging time correction is assumed for the vertical plume spread values.

For transient releases, the predicted concentration values are estimated using the three minute average horizontal plume spread values. Since the transient release can be of the order of several minutes, the conversion factor given in Equation B.178 is not suitable for the prediction of hourly concentration values. For transient releases, the hourly average concentrations are estimated from:

$$\chi_{60} = \frac{1}{3600} \int_{t-3600}^t \chi_3(x, t) dt \quad (\text{B.179})$$

where: t = time given in seconds
 χ_{60} = hourly (60 minute) average concentration
 χ_3 = three minute average concentration (assumed to be instantaneous)

For times prior to the release ($t < 0$ s), χ_3 is assumed to equal zero.

B1.6 Model Limitations

Before applying any model to solve a specific problem, it is important to recognize the limitations imposed by the model assumptions. The following have been identified as limitations to consider when applying GASCON:

- *Limited Pipeline Release Scenarios.* GASCON can only evaluate End Pipe Ruptures (Figure B.5) or release scenarios which can be considered as the superposition of two or more End Pipe Rupture cases. For example, the model does not currently contain the refinements to evaluate a short rupture located in the middle of a pipeline segment.
- *Upwind and Downwind Horizontal Jets.* The model cannot evaluate horizontal releases which are oriented at some arbitrary angle to the wind (e.g., crosswind releases).
- *Combustion Module Gas Chemistry.* The chemistry and physics of the ignited plume assume the sour gas to be comprised of methane (CH_4), carbon dioxide (CO_2) and H_2S only. Other gases are accounted for in a limited fashion by the heat of combustion factor. Caution should be exercised in applying the model to sour gas streams (for ignited cases only) whose composition differs significantly from that assumed by the model.
- *No Condensation Effects.* The model does not consider the dispersion and deposition of condensate aerosol clouds. Condensate is defined as a mixture of pentanes and heavier hydrocarbons which is a vapour in the formation and a liquid at atmospheric conditions.

The dispersion sub-models incorporate assumptions which can restrict their use to the following conditions:

- *Ensemble Average Concentrations.* Only mean concentrations are estimated. The model does not currently have the capability of predicting concentration fluctuations which can produce peak short-term (a few seconds) values.

- *Centreline Concentrations.* The model only predicts ground level concentration values below the plume centreline. The model does not currently have the capability to predict off axis values (which are less than the centreline values).
- *Travel times less than a few hours.* During periods characterized by light winds, disorganized and recirculating wind flows, the usefulness of dispersion models at distances beyond 10 km is limited (Mahoney and Spengler, 1975). A wind speed of 1 m/s (3.6 km/h) and a distance of 10 km corresponds to a travel time of 3 hours.
- *Averaging periods ranging from a few minutes to a few hours.* All the models presented are based on steady state meteorological assumptions (which are typically assumed to exist for either 3 minute to 1 hour periods). For longer averaging periods it is unlikely that the natural variability of the atmosphere will allow a given set of meteorological conditions to persist for periods of more than a few hours.
- *Flat terrain conditions.* Significant topographical features can have blocking, steering, channeling, or deflecting effects on the plume trajectory. The presence of elevated terrain can affect the height of the plume above the ground and can increase the level of turbulence over what would be expected for flat terrain. Moderately rough terrain can be accounted for adopting in appropriate surface roughness (Z_o) value.
- *Homogeneous terrain.* The models do not address changes in the surface roughness with varying downwind distances. Major surface discontinuities such as the presence of an urban area or large body of water are not addressed. These can produce their own local scale circulation systems. Areas where major surface discontinuities are present may be evaluated by varying the Z_o parameter for different model runs.
- *Steady State Atmospheric Conditions.* The models do not address transient atmospheric phenomena such as the rapid mixing of a plume above the mixing layer by the growth of the mixing height (sometimes called inversion breakup fumigation) or changes in wind direction.

The above mentioned limitations for the Passive Dispersion Module apply to nearly all dispersion models. Many are a result of the inherent uncertainties in describing the behavior of the atmosphere (e.g., *Ensemble average concentrations, Travel times less than a few hours and Averaging periods ranging from a few minutes to a few hours*).

For some cases where a model limitation may be an important factor, some indication of ground level concentrations can be obtained by running the model for different cases which bracket the case to be evaluated. For example the following limitations may be addressed in this manner: *Upwind and Downwind Horizontal Jets, Limited Pipeline Release Scenarios and Homogeneous Terrain Conditions*.

Models, especially "official" regulatory models, are sometimes extrapolated to conditions beyond those for which the model was developed when no other modelling approaches are available. It is the responsibility of the user to ensure that the models are applied correctly and to note any questionable extrapolations.

Appendix C
SIMPLE GAUSSIAN MODEL EVALUATION

C SIMPLE GAUSSIAN MODEL EVALUATION

C1.1 Introduction

A simple Gaussian dispersion plume model was used to predict plume centreline SF₆ concentrations. The predicted values were then compared to the observed values that were obtained from each traverse. The traverse data was evaluated rather than the stationary data as the stationary data was typically off the centreline. To arrive at observed concentration values two methods were used, one based on the Gaussian distribution from the Moment method and the other one based on the Concentration Maximum method. Each method provided one maximum concentration value for each traverse. To arrive at the predicted concentration values five different options were used and these are discussed in Section C1.3.

Paired versus Unpaired Data

The time of each traverse was known, therefore, a block of 3-min meteorological data could be attached to that traverse. This resulted in an observed value in time and space, ie. **paired**. Of course if no meteorological data existed (due to equipment failure) for that 3-min block in time, then a **paired** comparison run could not be made. To avoid this problem an **unpaired** data set was looked at. This meant sorting the traverse information on its own and then running all meteorological data that existed during the traverse times through the model. Hanna (1985) stated that a large data set should be paired when doing model evaluations. The US EPA (Cox 1988) protocol is based on unpaired data analysis. Both approaches have merit so to deal with this issue an evaluation of both paired and unpaired data were made.

Statistics Tables

Comparisons of the observed paired and unpaired data (in time and space), to predictions were made and many statistics were computed. The statistics are discussed further in Section C1.4 however two key modelling statistics were focused on for this evaluation. They were the "paired Hanna's M" and the "unpaired fractional bias" (US EPA - Cox 1988).

It was also helpful to key in on certain factors such as the (median P/median O) ratio. Models such as the Gaussian predict ensemble means and one might assume that mean values should be compared, however, since the means were not always normally distributed the median ratio was considered to be the significant value to focus on. To deal with this issue both medians and means appear in the summary tables.

Graphical Presentation

The **factor of two** analysis was another statistical approach looked at. These values appear in the summary tables and also in graphical form for all of the paired data runs. For the graphical presentation there are six small plots that appear on each page. The left hand side of the page is for "all possible cases" and the right hand side of the page is only for stable/low wind speeds (less than 3 m/s).

The top two plots are essentially a scatter plot of predicted over observed (P/O), only sorted. The log to the base 2 ($\log_2 P/O$) was chosen to ensure that the values fit on the graph and so that a value of ± 1 indicated a value of ± 2 . The middle plots provide the same information only as a function of windspeed. They provide a good measure of overprediction and underprediction. The middle plot for stable wind speeds (less than 3 m/s) was plotted to investigate what happened in that region. The bottom set of plots shows the **factor of two** analysis.

The following sections provide further details regarding the above issues. Section C1.2 and C1.3 covers the simple Gaussian model formulations and options. Section C1.4 covers the performance measures. Section C1.5 and C1.6 will cover the paired and unpaired data set statistics, respectively.

C1.2 Simple Gaussian Model - Formulations

SF₆ concentrations, χ (ppt), are predicted from the generic Gaussian relationship:

$$\chi = \frac{Q \cdot 10^{12}}{\pi \sigma_y \sigma_z U} \exp\left(-\frac{H^2}{2\sigma_z^2}\right) \quad (C.1)$$

where:

Q = SF₆ release rate (m³/s)
 σ_y = lateral plume standard deviation (m)
 σ_z = vertical plume standard deviation (m)
 U = wind speed at plume height (m/s)
 H = plume height (m)

For ground releases, the 4 m level wind speeds were used and for elevated releases, the 10 m level wind speeds were used. For ground releases, the plume height was taken as 1 m and for elevated releases, the plume height was estimated from momentum plume rise considerations. For neutral conditions, the plume height is given by:

$$H = h_s + \frac{6V_s R_s}{U} \quad (C.2)$$

For stable conditions, the plume height is taken as the minimum of the neutral value or the stable value predicted by:

$$H = h_s + 1.5 \left[\frac{V_s^2 R_s^2}{US^{1/2}} \right]^{1/3} \quad (C.3)$$

where:

h_s = fan height (2.3 m)
 V_s = fan exit velocity (m/s)
 R_s = fan radius (0.369 m)
 U = 10 m wind speed (m/s)
 S = stability parameter given by
 $S = \frac{g}{T} \left(\frac{\partial T}{\partial Z} + \Gamma \right)$

where:

g = acceleration due to gravity (9.81 m/s²)
 T = ambient temperature at 2 m (K)
 $\partial T / \partial Z$ = vertical temperature gradient 2 to 25 m (K/m)
 Γ = adiabatic temperature gradient 0.0098 (K/m)

These formulations amount to what was called the simple Gaussian model.

C1.3 Model Comparison - Options

Five sets of plume spread data were used in the simple concentration model (Equation 2.1). These include:

- **Option 1** (Field σ_{yi})

σ_{yi} = observed value based on Moment method

$\sigma_{zi} = 0.3 \sigma_w x / U$ (similar to Equation 7.4 in Volume 1)

- **Option 2** (Field σ_{yi})

σ_{yi} = observed value based on Concentration Maximum method

$\sigma_{zi} = 0.3 \sigma_w x / U$ (similar to Equation 7.4 in Volume 1)

- **Option 3** (Field σ_v)

$\sigma_{yi} = 0.3 \sigma_v x / U$ (Equation 7.4 in Volume 1)

$\sigma_{zi} = 0.3 \sigma_w x / U$ (similar to Equation 7.4 in Volume 1)

- **Option 4** (Field σ_v)

$\sigma_{yi} = 0.3 \sigma_v x WDE / U$ (Equation 7.7 in Volume 1)

$\sigma_{zi} = 0.3 \sigma_w x / U$ (similar to Equation 7.4 in Volume 1)

- **Option 5** (Alberta Environment σ)

$\sigma_{yc} = ax^{0.88}$ (Equation 7.16 in Volume 1)

$\sigma_{zc} = bx^c$ (similar to Equation 7.16 in Volume 1)

The first two methods are based on using the observed value of σ_{yi} as collected in the field by both the Moment and Concentration Maximum methods. The third and fourth methods are based on using field meteorology without accounting for, and then accounting for wind direction shear. The fifth method is based on using the composite time-averaged (3-minute) Alberta Environment plume spread formulations σ_{yc} for a surface roughness of $Z_o=1.0$ cm. For the fifth case, the stability class was determined from a STAR analysis of Calgary International Airport data, where the constants, (a, b and c), are a function of stability class:

Stability Class	D	E	F
a	0.125	0.0916	0.0623
b	0.1077	0.077	0.0623
c	0.81	0.78	0.72

Options one to five range from maximum to minimum use of on-site data and provide a measure of the simple Gaussian formulation to predict the observed SF₆ concentrations.

Since Option 5 used the existing regulatory sigmas (Alberta Environment) and provided the a reasonable overall performance, further analysis was completed by splitting the Option 5 case into ground and elevated. Another case was also developed that allowed σ_{yc} and σ_{zc} to have a smaller averaging time of 30 seconds and that case was split into ground and elevated as well.

Table C.1 outlines all the **paired** cases that were run:

Table C.1
Summary of all Paired Cases Run

	Option	Stable	Figure No.	Table No.	Table No.	σ_y	σ_z	Average Time
		<3 m/s	Moment	Conc Max	Moment			
	1 all cases	Yes	C.1	C.2	C.2	σ_{yi}	σ_{zi}	I
	2 all cases	"	C.2	C.2	C.2	σ_{yi}	σ_{zi}	I
	3 all cases	"	C.3	C.2	C.2	σ_{yi}	σ_{zi}	I
	4 all cases	"	C.4	C.2	C.2	σ_{yi}	σ_{zi}	I
AE	5 all cases	"	C.5	C.2	C.2	σ_{yc}	σ_{zc}	3-min
AE	5 ground	"	C.6	C.4	C.4	σ_{yc}	σ_{zc}	3-min
AE	5 elevated	"	C.7	C.4	C.4	σ_{yc}	σ_{zc}	3-min
AE	5 all cases	"	C.8	C.4	C.4	σ_{yc}	σ_{zc}	30-sec
AE	5 ground	"	C.9	C.4	C.4	σ_{yc}	σ_{zc}	30-sec
AE	5 elevated	"	C.10	C.4	C.4	σ_{yc}	σ_{zc}	30-sec

The **unpaired** analysis was done on Option 5 only for ground and elevated cases.

C1.4 Performance Measures

The performance of the simple Gaussian model was evaluated using standard statistical and graphical procedures. Considerable effort has been made to determine the appropriate performance measures for dispersion models (Hanna 1975, Cox 1988). A wide variety of performance indices have been suggested since it is difficult to arrive at a single quantitative index of accuracy. Unfortunately there is a temptation to get carried away and compute a multitude of statistical measures and comparisons which can make it even more difficult to arrive at the bottom line answer on "How well does the model work?".

Performance measures can be obtained from observed and predicted data sets that are either paired or unpaired in time and/or space. If a large data base exists and the goal is to obtain an understanding of model physics, then paired data sets are preferable. If the model performance is to be compared to the ability of the model to predict maximum values for regulatory purposes, then unpaired data sets can be used. The US EPA (Cox 1988) protocol for screening and testing a model for regulatory use is based on unpaired data.

For the evaluation of the simple Gaussian model, the following parameters were calculated for each set of observed and predicted data sets:

- Mean observed ($\bar{O}$) and predicted ($\bar{P}$) concentrations. The ratio of mean predicted to observed ($\bar{P}/\bar{O}$ and $\bar{P}/\bar{O}$). For perfect agreement $\bar{O} = \bar{P}$ and $\bar{P}/\bar{O} = \bar{P}/\bar{O} = 1.0$.
- Median observed ($\tilde{O}$) and predicted ($\tilde{P}$) concentrations. The ratio of mean predicted to observed ($\tilde{P}/\tilde{O}$ and $\tilde{P}/\tilde{O}$). For perfect agreement $\tilde{O} = \tilde{P}$ and $\tilde{P}/\tilde{O} = \tilde{P}/\tilde{O} = 1.0$.
- The average bias which is defined from:

$$\bar{d} = \frac{\sum (O_i - P_i)}{N}$$

which like $\bar{P}/\bar{O}$, $\bar{P}/\bar{O}$, $\tilde{P}/\tilde{O}$ and $\tilde{P}/\tilde{O}$ will indicate whether the model generally over or underpredicts. For perfect agreement $\bar{d} = 0.0$.

- The Pearson product-moment correlation coefficient:

$$r = \frac{\sum (O_i - \bar{O})(P_i - \bar{P})}{\sqrt{\sum (O_i - \bar{O})^2 \sum (P_i - \bar{P})^2}}$$

which presumes a linear relationship between O_i and P_i . This correlation coefficient should be used as a measure of relative rather than absolute measure of model performance. For example, in a recent EPRI model development project, an improved model resulted in an r value of 0.58, a significant improvement over the CRSTER model value of 0.14 (Ventekram 1988). For perfect agreement $r = 1.0$.

- The slope (S) and intercept (B) obtained from a least squares fit of P_i as function of O_i . This method presumes a linear relationship between P_i and O_i . For perfect agreement $\bar{B} = 0$ and $\bar{M} = 1.0$.
- The relative mean absolute error (RMAE) was computed from:

$$RMAE = \frac{\sum |O - P|}{N\bar{O}}$$

For perfect agreement RMAE = 0.0

- The mean relative error (MRE) was computed from:

$$MRE = \left\{ \frac{2}{N} \sum \left(\frac{|P_i - O_i|}{|P_i + O_i|} \right)^2 \right\}^{1/2}$$

For perfect agreement MRE = 0.0

- Percent of predictions within a specified factor of the observation. For this evaluation, the specified factors are 2 and 3. Ideally, perfect agreement would give 100% within these factors.
- Hanna's (1975) dimensionless mean square error (M) from:

$$M = \frac{\overline{(P - O)^2}}{(\bar{P}\bar{O})}$$

A lower value of M indicates a better model. The method gives larger concentrations more weight because the difference $\bar{P} - \bar{O}$ will be influenced by the larger concentrations. A perfect model would have an M value of zero; the best available models have M values of order 1. Models with poor performance have high M values.

The above statistical performance measures were applied to paired data sets. For unpaired data sets, the cumulative frequency distributions of the normalized predicted and observed concentrations are presented graphically. The US EPA suggests that the fractional bias (FB) be calculated from unpaired data.

$$FB = 2 \frac{(\bar{O} - \bar{P})}{(\bar{O} + \bar{P})}$$

where $\bar{O}$ and $\bar{P}$ refer to the 25 highest observed and predicted values.

The previously discussed performance measures were applied to the traverse data obtained from the Field Measurement Program. While these measures are by no means complete, they will provide a preliminary evaluation on the ability of simple Gaussian model to predict plume centreline concentrations.

C1.5 Model Performance - Paired Data

Summary Table of Statistics

Table C.2 presents the performance statistics for different combinations of the observed and predicted data sets. The results from the table indicates the following:

- The poorest performance of all the options was with Option 4. The model generally underpredicts. This option incorporated a wind direction shear enhancement term in the estimation of σ_{yi} . This increased σ_{yi} and decreased the predicted concentrations.
- For the other options, there is no one option which stands out as being the best. Generally speaking, the best performances were obtained when the predictions were compared to the observations based on the Moment method.

For example: the minimum bias is associated with Option 5; the maximum correlation coefficient (r) with the Option 1 predictions; the maximum percentage within a factor of 2 with the Option 2 predictions and the maximum percentage within a factor of 3 with the Option 1 prediction. The minimum Hanna M values are associated with Option 2 and 5 predictions.

Table C.3 presents the performance statistics for a subset of the available data set. Specifically, the subset includes:

- Ground Releases when the 4 m level tower wind speed was less than 3 m/s and when Calgary airport observations indicated a Pasquill-Gifford stability class E or F. The number of traverses that meet these criteria is 191 compared to the 704 in the full data set.
- Elevated releases when the 10 m level tower wind speed was less than 3 m/s and when Calgary airport observations indicated a Pasquill-Gifford stability class E or F. The number of traverses that meet this criteria is 119 compared to the 704 in the full data set.

From the table, the following comments can be derived:

- For ground releases, the simple Gaussian model on the average underpredicts for all options. Options 1, 2 and 3 show a general improvement of predictions within a factor of 2 and 3. For Options 3 and 4, the percentage decreases.

Table C.2

Comparison of Model Performance Statistics.

	MEAN O	MEAN P	MEAN P O	MEAN P MEAN O	MEDIAN O	MEDIAN P	MEDIAN P O	MEDIAN P O	MEDIAN P MEDIAN O	AVG. BIAS (P vs. O)	r (P vs. O)	SLOPE	INTERCEPT	RMAE	MRE	% WITHIN FACTOR OF 2	% WITHIN FACTOR OF 3	HANNA'S M
OPTION 1 Moment Maximum	1304 1561	1040 1040	0.82 0.66	0.80 0.67	902 1069	769 769	0.77 0.66	0.85 0.72	262 518	0.43 0.40	0.36 0.27	580 624	0.65 0.65	0.68 0.69	50 47	68 64	35.6 116.7	
OPTION 2 Moment Maximum	1304 1561	1234 1234	0.97 0.79	0.95 0.79	902 1069	878 878	0.90 0.74	0.97 0.82	67 324	0.39 0.44	0.38 0.35	747 698	0.70 0.66	0.69 0.67	51 51	67 67	2.0 38.5	
OPTION 3 Moment Maximum	1304 1561	1167 1167	0.94 0.76	0.90 0.75	902 1069	810 810	0.85 0.72	0.90 0.76	135 391	0.27 0.29	0.26 0.23	838 823	0.79 0.73	0.71 0.70	43 45	63 63	8.4 59.3	
OPTION 4 Moment Maximum	1304 1561	573 573	0.39 0.32	0.44 0.37	902 1069	337 337	0.42 0.35	0.37 0.32	729 985	0.19 0.21	0.12 0.11	426 410	0.79 0.78	0.82 0.85	29 27	50 46	501.5 766.0	
OPTION 5 Moment Maximum	1304 1561	1304 1304	1.17 0.95	1.0 0.84	902 1069	859 859	1.05 0.89	0.95 0.80	-2 254	0.23 0.24	0.26 0.22	1055 1054	0.71 0.70	0.80 0.75	42 41	58 60	3.5 3.0	

O = Observed centreline SF₆ concentration (ppt) for the moment or concentration maximum method.

P = Predicted centreline SF₆ concentration (ppt) from one of Option 1 to 5 (Options 1 to 4 assume instantaneous plume spreads, while Option 5 assumes a 3 minute average plume spread).

Table C.3

Comparison of Model Performance Statistics for Low Wind Speed Stable Conditions.

	All Cases			Stable Ground $U_s < 3$ m/s			Stable Elevated $U_{10} < 3$ m/s		
	$\frac{MedianP}{MedianO}$	% Within Factor of 2	% Within Factor of 3	$\frac{MedianP}{MedianO}$	% Within Factor of 2	% Within Factor of 3	$\frac{MedianP}{MedianO}$	% Within Factor of 2	% Within Factor of 3
OPTION 1 Moment Maximum	0.85 0.72	50 47	68 64	0.38 0.34	51 42	79 69	3.01 2.49	29 32	47 48
OPTION 2 Moment Maximum	0.97 0.82	51 51	67 67	0.43 0.39	55 52	80 79	3.45 2.84	29 29	43 47
OPTION 3 Moment Maximum	0.90 0.76	43 45	63 63	0.40 0.35	25 28	59 52	3.17 2.62	27 32	39 47
OPTION 4 Moment Maximum	0.37 0.31	29 27	50 46	0.17 0.15	17 15	38 35	1.32 1.09	33 35	59 60
OPTION 5 Moment Maximum	1.19 1.01	42 41	58 60	0.53 0.47	51 55	70 70	4.22 3.49	22 24	34 44

O = Observed centreline SF_e concentration (ppt) for the moment or concentration maximum method.P = Predicted centreline SF_e concentration (ppt) from one of Option 1 to 5 (Options 1 to 4 assume instantaneous plume spreads, while Option 5 assumes a 3 minute average plume spread).

One of the difficulties with a ground release is that the Gaussian approximation in the vertical may not be valid. This is why alternate dispersion models have been developed for surface releases. For example, Horst (1979) assumed the vertical spread is exponential rather than Gaussian.

- For elevated releases, the simple Gaussian model overpredicts by a factor of about 3 for all options except for Option 4. For Option 4, the median P over median O ratio indicates relatively good agreement.

Option 4 includes wind direction shear enhancement in the estimation of the crosswind spread. The improvement in model performance for this meteorological subset may indicate that wind shear enhanced dispersion is important for low wind, stable conditions.

Graphical Presentation - Factor of Two Analysis

Figures C.1 to C.7

These plots serve as a useful visual aid to depict how well the model was doing. Figures C.1 to C.5 are for Options 1 to 5 with Figures C.6 and C.7 breaking Option 5 into ground and elevated. Note that Option 5 used 3-minute sigma values for these first seven plots. Visually the best performance appears to have been with Option 1. Options 2, 3 and 4 were underpredicting while Option 5 first overpredicting until it was further broken into ground and elevated. The elevated case then switched to underprediction. (Note the plots say surface rather than ground but they mean the same thing). The ground under the same condition overpredicted up to around 1.5 m/s and then underpredicted. The conclusion drawn after a review of these first plots was that any further model evaluations should split the analysis into ground and elevated.

Figures C.8 to C.10

To ensure that the model was predicting as close to instantaneous as possible sigma values of 30-second averaging time were incorporated. Figures C.8, C.9 and C.10 are the "all possible cases", ground and elevated, respectively. Table C.4 provides the statistics similar to the format in the earlier Table C.2.

The **factor of two** performance drops for the elevated stable < 3 m/s as before. There is some improvement in the **factor of two** performance for "all cases" but only a few percentage points. The median P/median O ratio for "all cases" shows slight overprediction as it did before.

The averaging time change will shift the results to overpredict more. This is seen by Figure C.9 particularly as the overprediction is now for wind speeds less than 2.5 m/s when it was 1.5 m/s using the 3-minute sigmas. Even larger overpredictions for the elevated are found with a median P/median O ratio of 7.8.

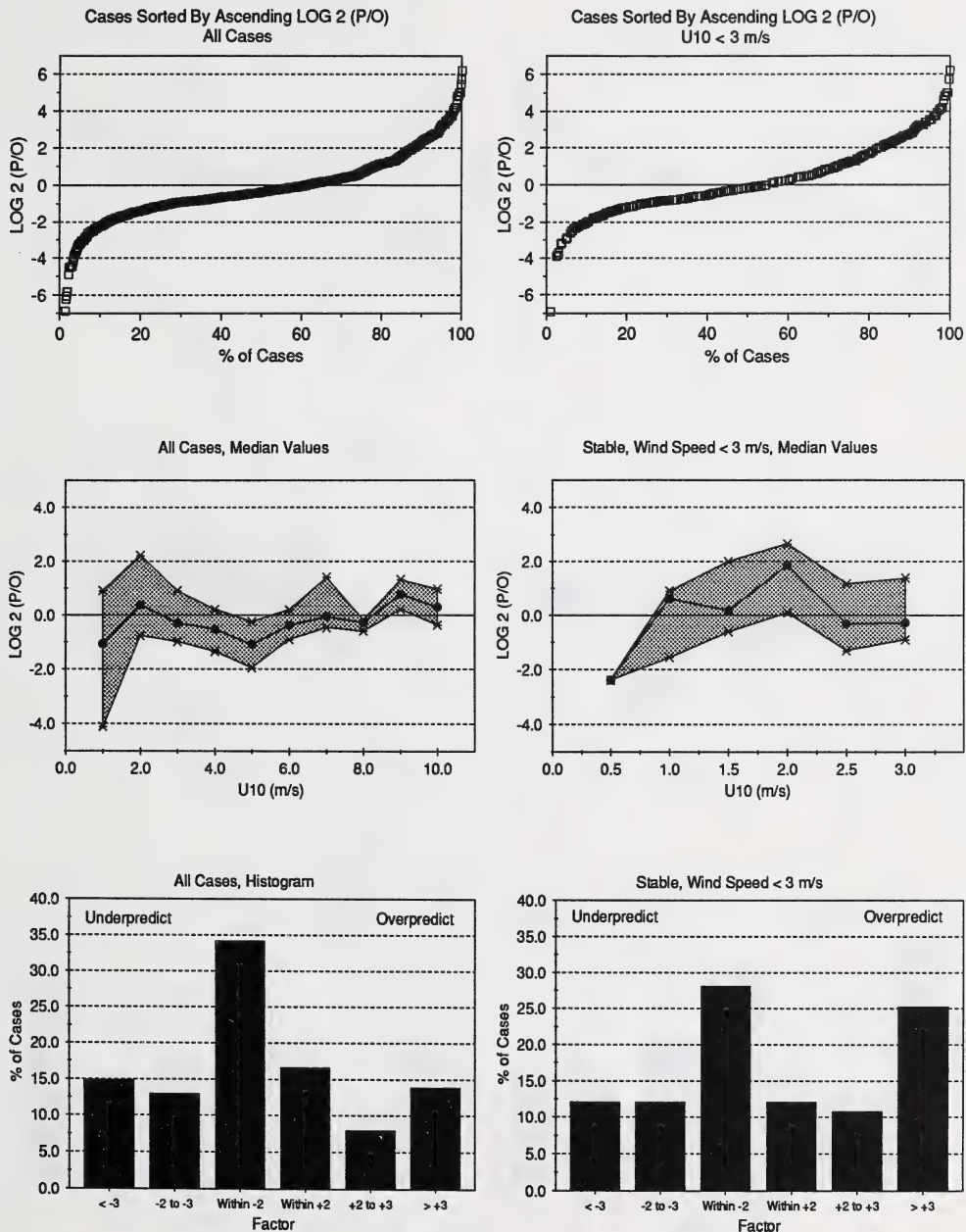


Figure C.1

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 1 (Instantaneous). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

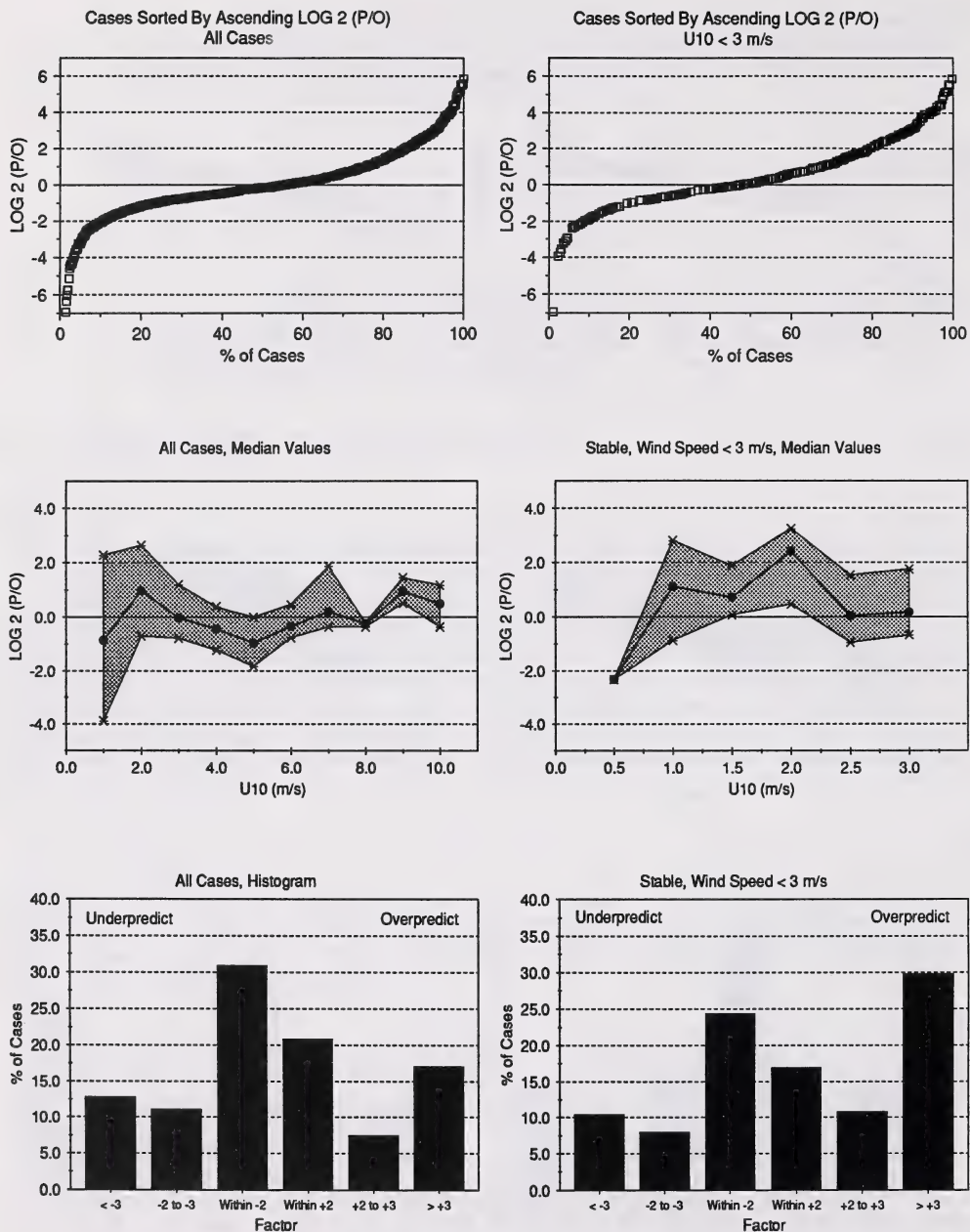


Figure C.2

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 2 (Instantaneous). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

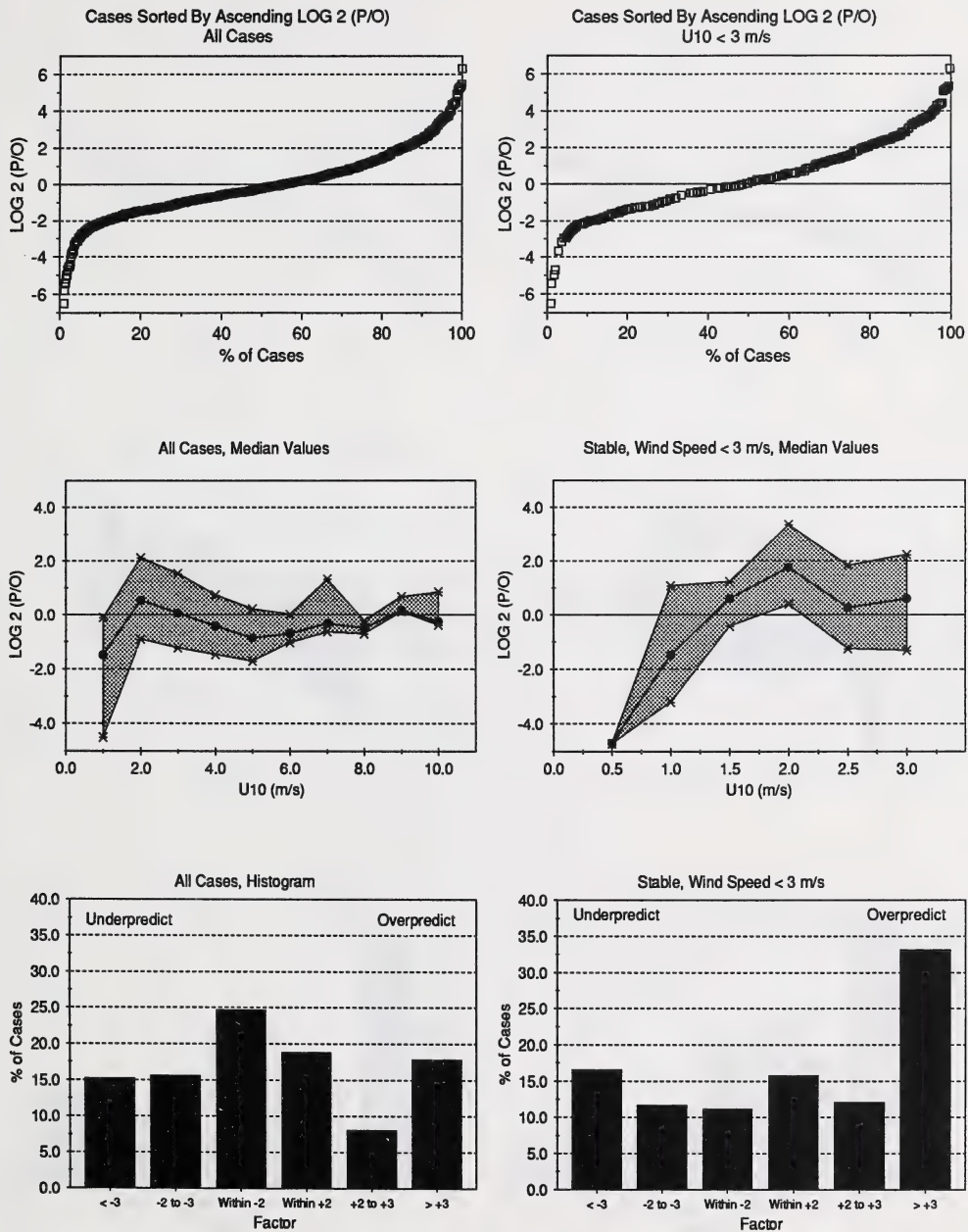


Figure C.3

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 3 (Instantaneous). The Shaded Envelope Indicates the 25 and 75 Percentile limits.

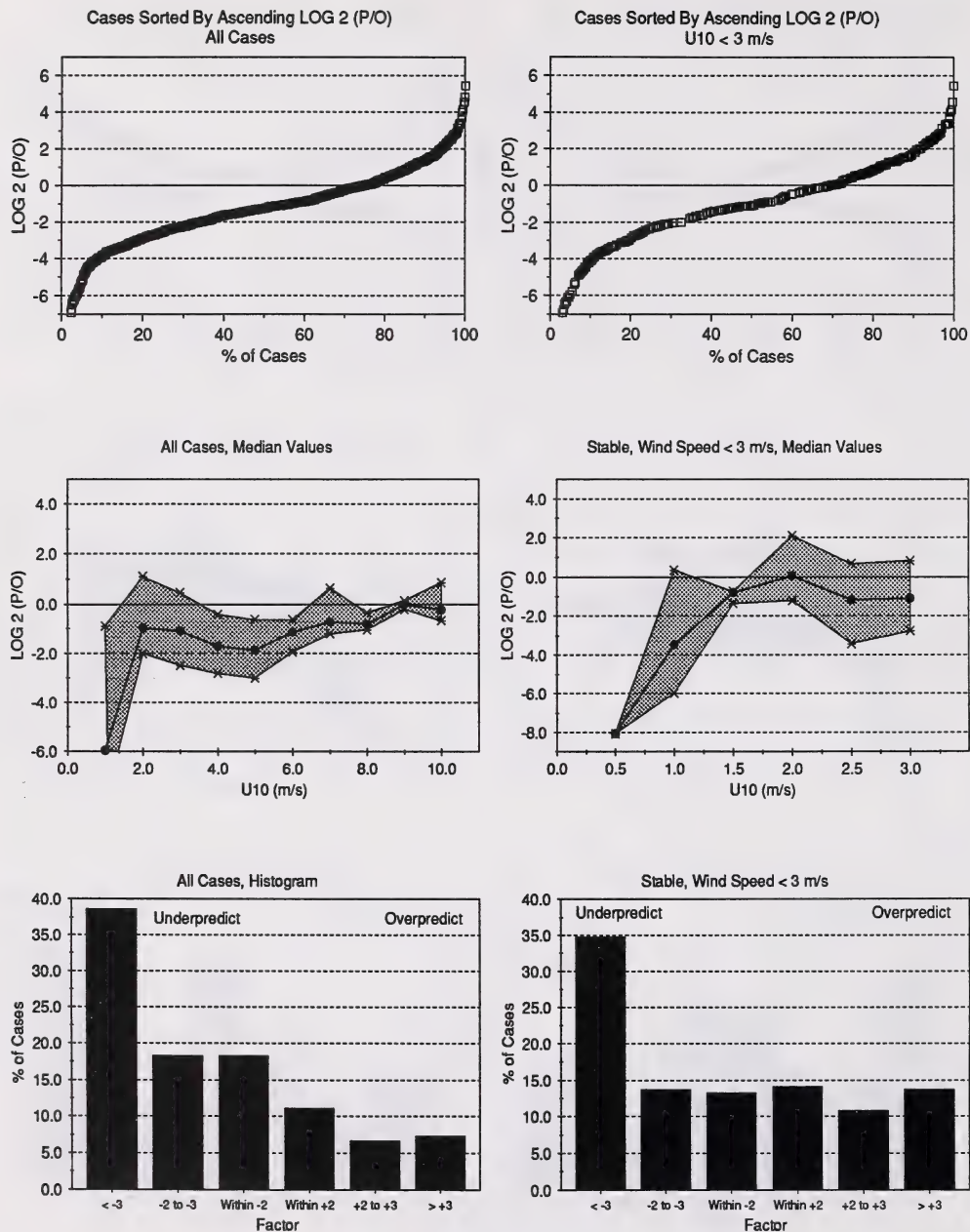


Figure C.4

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 4 (Instantaneous). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

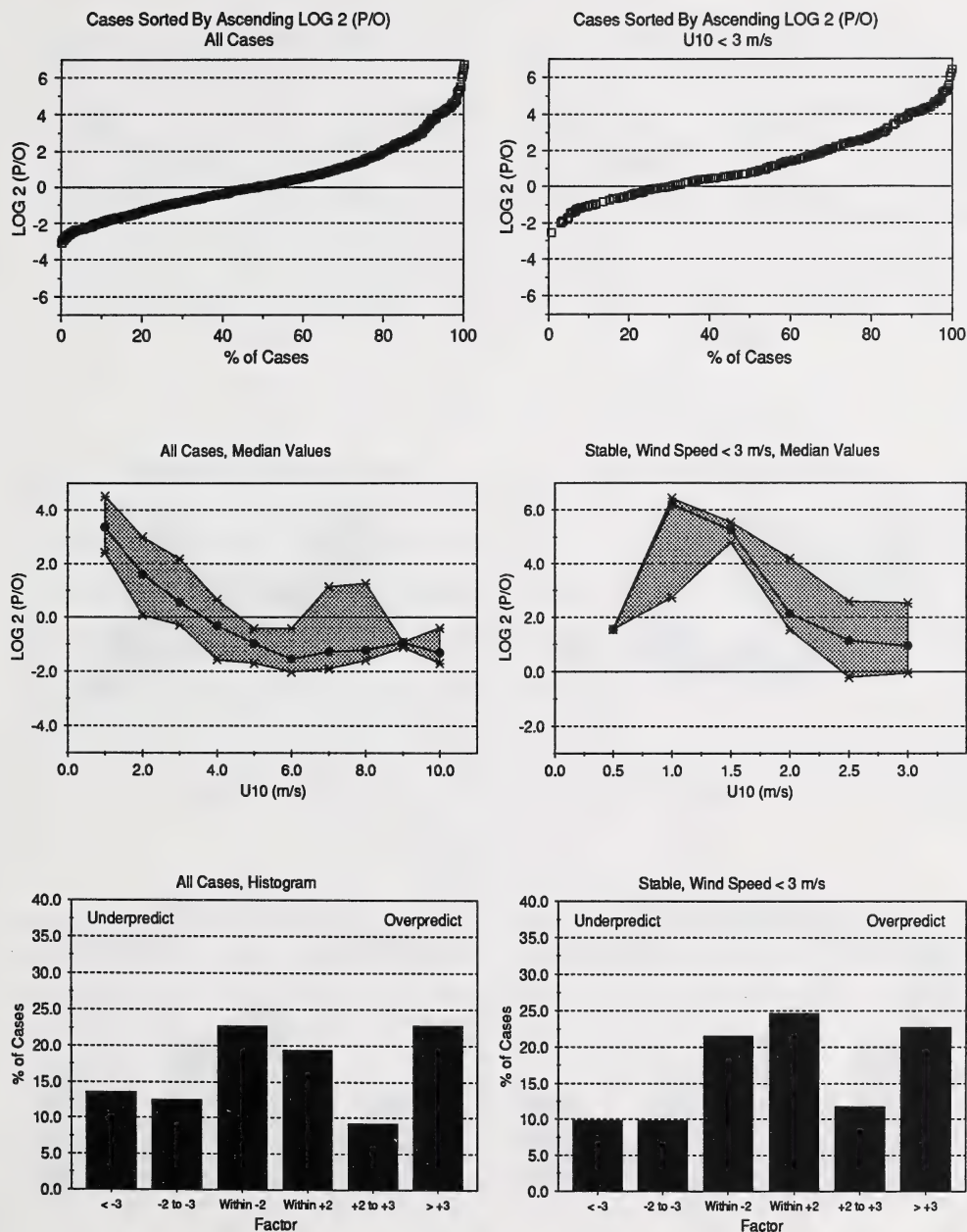


Figure C.5

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 5 (3 minute sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

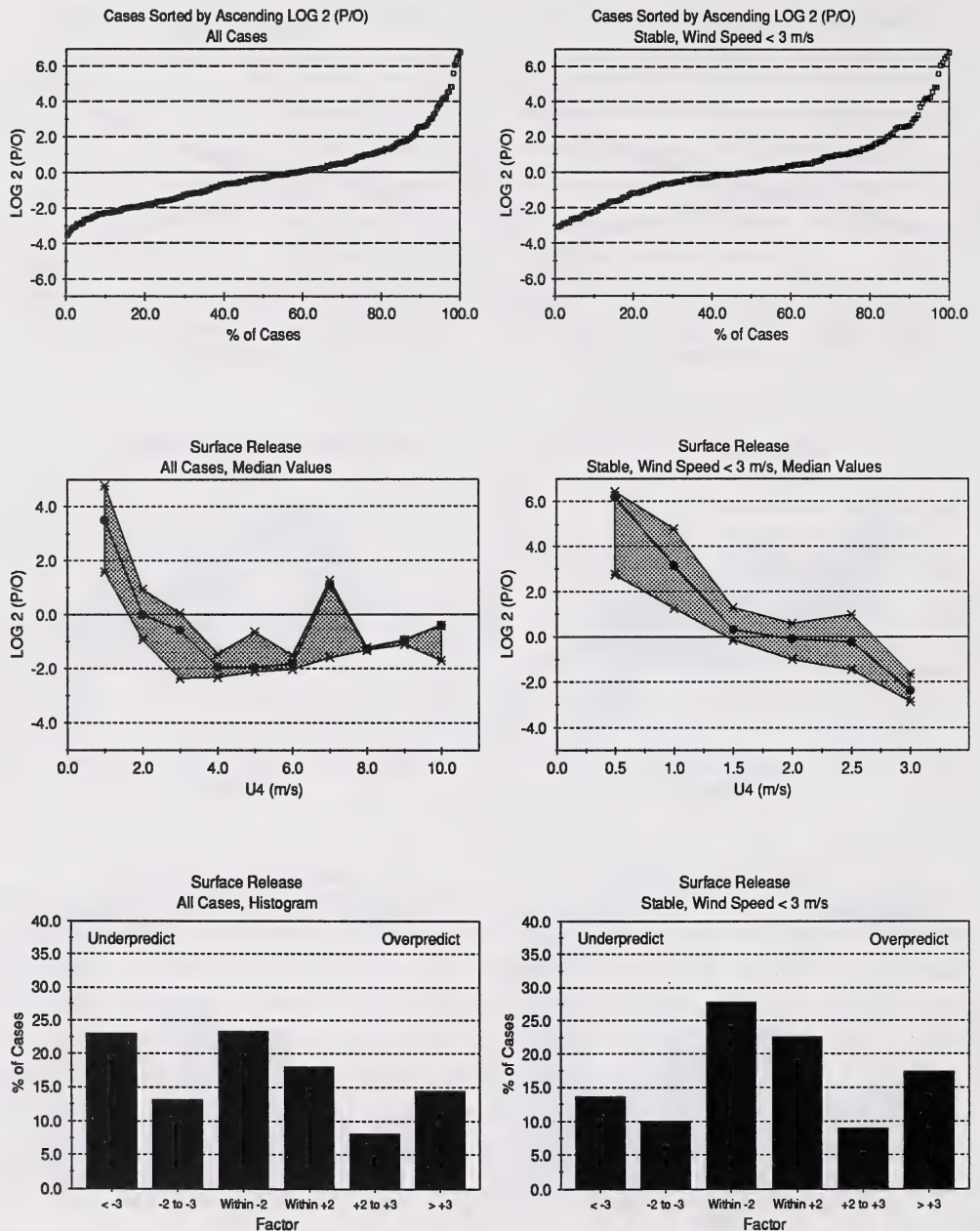


Figure C.6

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for Ground Releases and Stable, < 3 m/s for Option # 5 (3 minute sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

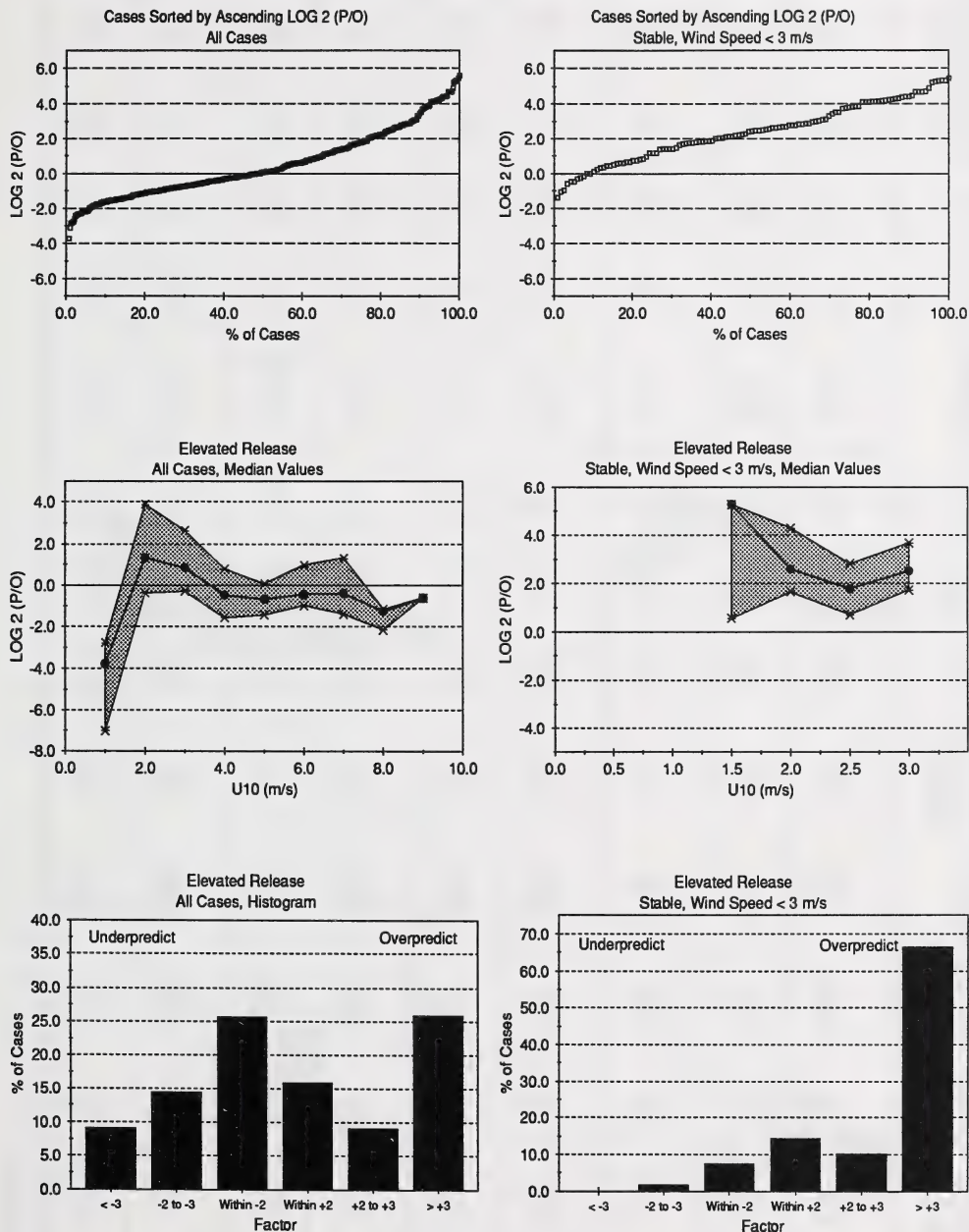


Figure C.7

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for Elevated Releases and Stable, < 3 m/s for Option # 5 (3 minute sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

Table C.4

Option 5 Statistics for Paired Ground and Elevated Releases. Both 30 Second and 3 Minute Sigmas are Included.

OPTION 5	MEAN $\frac{P}{O}$	MEAN $\frac{O}{P}$	MEAN $\frac{P}{O}$	MEAN $\frac{O}{P}$	MEDIAN $\frac{P}{O}$	MEDIAN $\frac{O}{P}$	MEDIAN P	MEDIAN O	MEDIAN $\frac{P}{O}$	MEDIAN $\frac{O}{P}$	$r(P \text{ vs. } O)$	AVG. BIAS	SLOPE	INTERCEPT	RMAE	MRE	% WITHIN FACTOR OF 2	% WITHIN FACTOR OF 3
Ground Release (All Cases) Moment Maximum	0.92 0.73	2028.5 2467.4	1839.8 1839.8	0.91 0.75	1.27 1.38	1850.0 2155.0	1528.6 1528.6	0.83 0.71	0.126 0.142	188.7 627.6	0.15 0.14	1541.9 1489.7	0.76 0.71	0.71 0.71	41.3 42.8	62.5 62.2		
Stable, $U_{10} < 3$ m/s Moment Maximum	4.79 3.31	2368.0 2917.2	2461.7 2461.7	1.04 0.84	0.96 0.83	2099.0 2431.0	2257.7 2257.7	1.08 0.93	-0.071 -0.053	-93.7 455.4	-0.09 -0.05	2666.0 2615.3	0.76 0.70	0.68 0.67	50.3 53.9	64.4 66.0		
Elevated Release (All Cases) Moment Maximum	3.83 2.80	812.4 946.5	943.2 943.2	1.16 1.0	1.02 0.91	657.0 775.0	756.8 756.8	1.15 0.98	0.094 0.060	-130.7 3.36	0.09 0.04	871.8 901.2	0.88 0.87	0.72 0.70	41.6 40.6	60.6 62.2		
Stable, $U_{10} < 3$ m/s Moment Maximum	9.04 6.23	504.9 624.5	1492.8 1492.8	2.96 2.39	5.35 4.13	255.0 309.0	1403.2 1403.2	5.50 4.54	0.250 0.261	-987.8 -868.2	0.26 0.22	965.4 959.8	2.16 1.68	0.94 0.87	21.9 24.4	31.1 37.8		
σ_1 (All cases) Moment Maximum	5.39 3.84	1303.6 1560.8	1865.4 1865.4	1.43 1.20	1.31 1.10	902.0 1069.0	1229.5 1229.5	1.36 1.15	0.250 0.261	-564.1 -307.5	0.37 0.32	1381.5 1373.4	1.00 0.86	0.72 0.69	43.6 44.3	61.7 62.9		
Ground Release (All cases) Moment Maximum	5.26 3.60	2028.5 2467.4	2632.7 2632.7	1.30 1.07	1.13 0.91	1850.0 2155.0	2187.4 2187.4	1.18 1.02	0.127 0.149	-604.2 -165.3	0.21 0.20	2206.5 2131.7	0.92 0.79	0.69 0.67	43.1 43.1	64.3 62.2		
Stable, $U_{10} < 3$ m/s Moment Maximum	6.86 4.74	2368.0 2917.2	3522.6 3522.6	1.49 1.21	1.38 1.18	2099.0 2431.0	3230.7 3230.7	1.54 1.33	-0.071 -0.053	-1154.6 -605.5	-0.12 -0.08	3815.0 3742.5	0.99 0.81	0.69 0.66	48.7 50.8	63.9 67.0		
Elevated Release (All cases) Moment Maximum	5.48 4.00	812.4 946.5	1349.6 1349.6	1.66 1.43	1.47 1.30	657.0 775.0	1083.0 1083.0	1.65 1.40	0.094 0.060	-537.2 -403.1	0.13 0.06	1247.5 1289.6	1.13 0.98	0.74 0.70	43.9 45.1	59.9 63.4		
Stable, $U_{10} < 3$ m/s Moment Maximum	12.94 8.92	504.9 624.5	2136.1 2136.1	4.23 3.42	7.66 5.91	255.0 309.0	2007.9 2007.9	7.87 6.50	0.193 0.183	-1631.2 -1511.6	0.31 0.24	1980.3 1984.7	3.30 2.56	1.03 0.96	15.1 17.7	23.5 28.6		

The first four rows are for 3-minutes sigmas.

The next five rows are for 30-seconds sigmas.

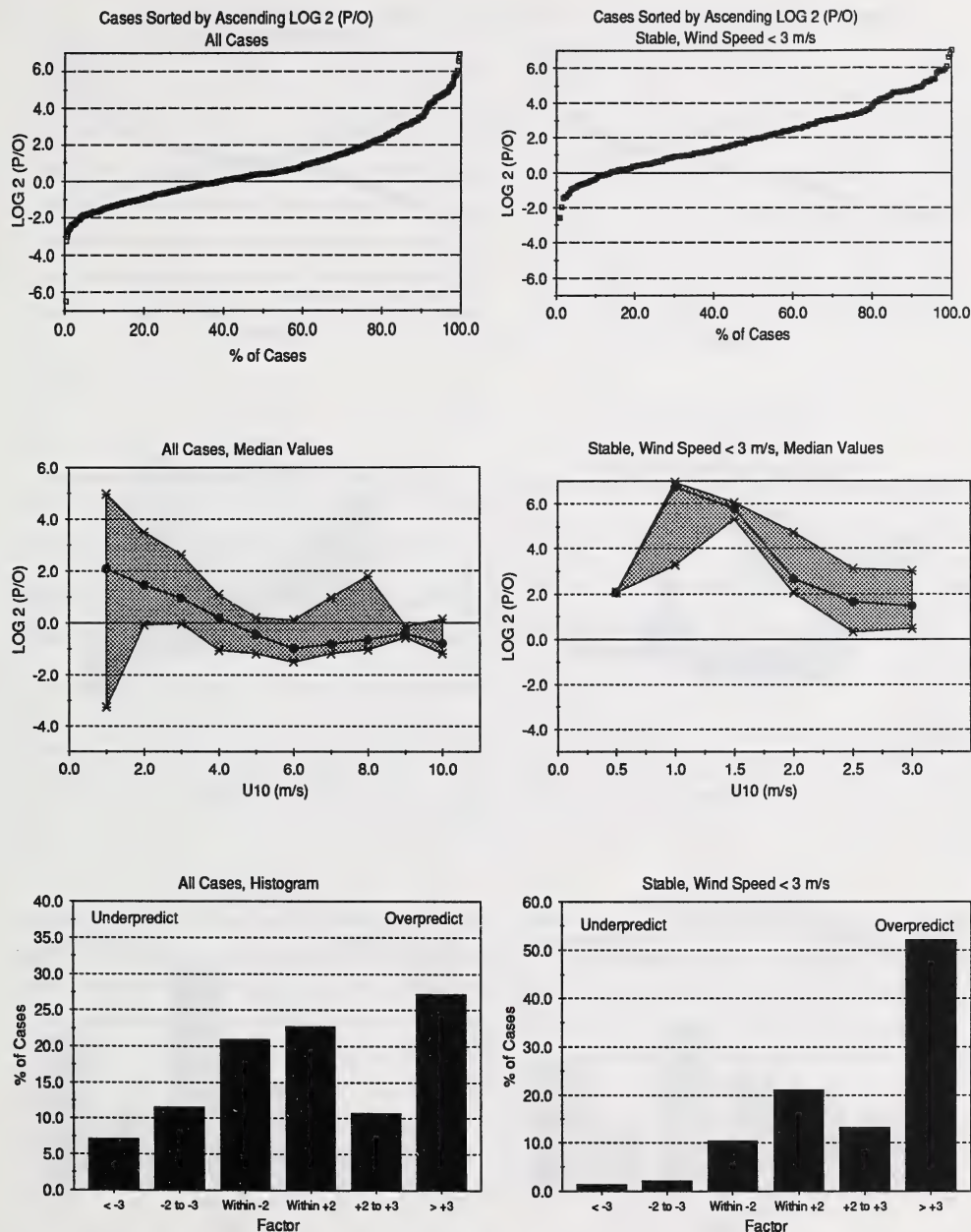


Figure C.8

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 5 (30 second sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

Table C.4

Option 5 Statistics for Paired Ground and Elevated Releases. Both 30 Second and 3 Minute Sigmas are Included.

OPTION 5	MEAN $\frac{P}{O}$	MEAN O	MEAN P	MEAN $\frac{P}{O}$	MEAN $\frac{P}{O}$	MEDIAN $\frac{P}{O}$	MEDIAN O	MEDIAN P	MEDIAN $\frac{P}{O}$	r(P vs. O)	AVG. BIAS	SLOPE	INTERCEPT	RMAE	MRE	% WITHIN FACTOR OF 2	% WITHIN FACTOR OF 3
Ground Release (All Cases) Moment Maximum	0.92 0.73	2028.5 2467.4	1839.8 1839.8	0.91 0.75	1.27 1.58	1850.0 2155.0	1528.6 1528.6	0.83 0.71	0.126 0.142	0.126 0.142	188.7 627.6	0.15 0.14	1541.9 1489.7	0.76 0.71	0.71 0.71	41.3 42.8	62.5 62.2
Stable, $U_{10} < 3$ m/s Moment Maximum	4.79 3.31	2368.0 2917.2	2461.7 2461.7	1.04 0.84	0.96 0.83	2099.0 2431.0	2257.7 2257.7	1.08 0.93	-0.071 -0.053	-0.071 -0.053	-93.7 455.4	-0.09 -0.05	2666.0 2615.3	0.76 0.70	0.68 0.67	50.3 53.9	64.4 66.0
Elevated Release (All Cases) Moment Maximum	3.83 2.80	812.4 946.5	943.2 943.2	1.16 1.0	1.02 0.91	657.0 775.0	756.8 756.8	1.15 0.98	0.094 0.060	0.094 0.060	-130.7 3.36	0.09 0.04	871.8 901.2	0.88 0.87	0.72 0.70	41.6 40.6	60.6 62.2
Stable, $U_{10} < 3$ m/s Moment Maximum	9.04 6.23	504.9 624.5	1492.8 1492.8	2.96 2.39	5.35 4.13	255.0 309.0	1403.2 1403.2	5.50 4.54	0.250 0.261	0.250 0.261	-987.8 -868.2	0.26 0.22	965.4 959.8	2.16 1.68	0.94 0.87	21.9 24.4	31.1 37.8
σ_1 (All cases) Moment Maximum	5.39 3.84	1303.6 1560.8	1865.4 1865.4	1.43 1.20	1.31 1.10	902.0 1069.0	1229.5 1229.5	1.36 1.15	0.250 0.261	0.250 0.261	-564.1 -307.5	0.37 0.32	1381.5 1373.4	1.00 0.86	0.72 0.69	43.6 44.3	61.7 62.9
Ground Release (All cases) Moment Maximum	5.26 3.60	2028.5 2467.4	2632.7 2632.7	1.30 1.07	1.13 0.91	1850.0 2155.0	2187.4 2187.4	1.18 1.02	0.127 0.149	0.127 0.149	-604.2 -165.3	0.21 0.20	2206.5 2131.7	0.92 0.79	0.69 0.67	43.1 43.1	64.3 62.2
Stable, $U_{10} < 3$ m/s Moment Maximum	6.86 4.74	2368.0 2917.2	3522.6 3522.6	1.49 1.21	1.38 1.18	2099.0 2431.0	3230.7 3230.7	1.54 1.33	-0.071 -0.053	-0.071 -0.053	-1154.6 -605.5	-0.12 -0.08	3815.0 3742.5	0.99 0.81	0.69 0.66	48.7 50.8	63.9 67.0
Elevated Release (All cases) Moment Maximum	5.48 4.00	812.4 946.5	1349.6 1349.6	1.66 1.43	1.47 1.30	657.0 775.0	1083.0 1083.0	1.65 1.40	0.094 0.060	0.094 0.060	-537.2 -403.1	0.13 0.06	1247.5 1289.6	1.13 0.98	0.74 0.70	43.9 45.1	59.9 63.4
Stable, $U_{10} < 3$ m/s Moment Maximum	12.94 8.92	504.9 624.5	2136.1 2136.1	4.23 3.42	7.66 5.91	255.0 309.0	2007.9 2007.9	7.87 6.50	0.193 0.183	0.193 0.183	-1631.2 -1511.6	0.31 0.24	1980.3 1984.7	3.30 2.56	1.03 0.96	15.1 17.7	23.5 28.6

The first four rows are for 3-minutes sigmas.

The next five rows are for 30-seconds sigmas.

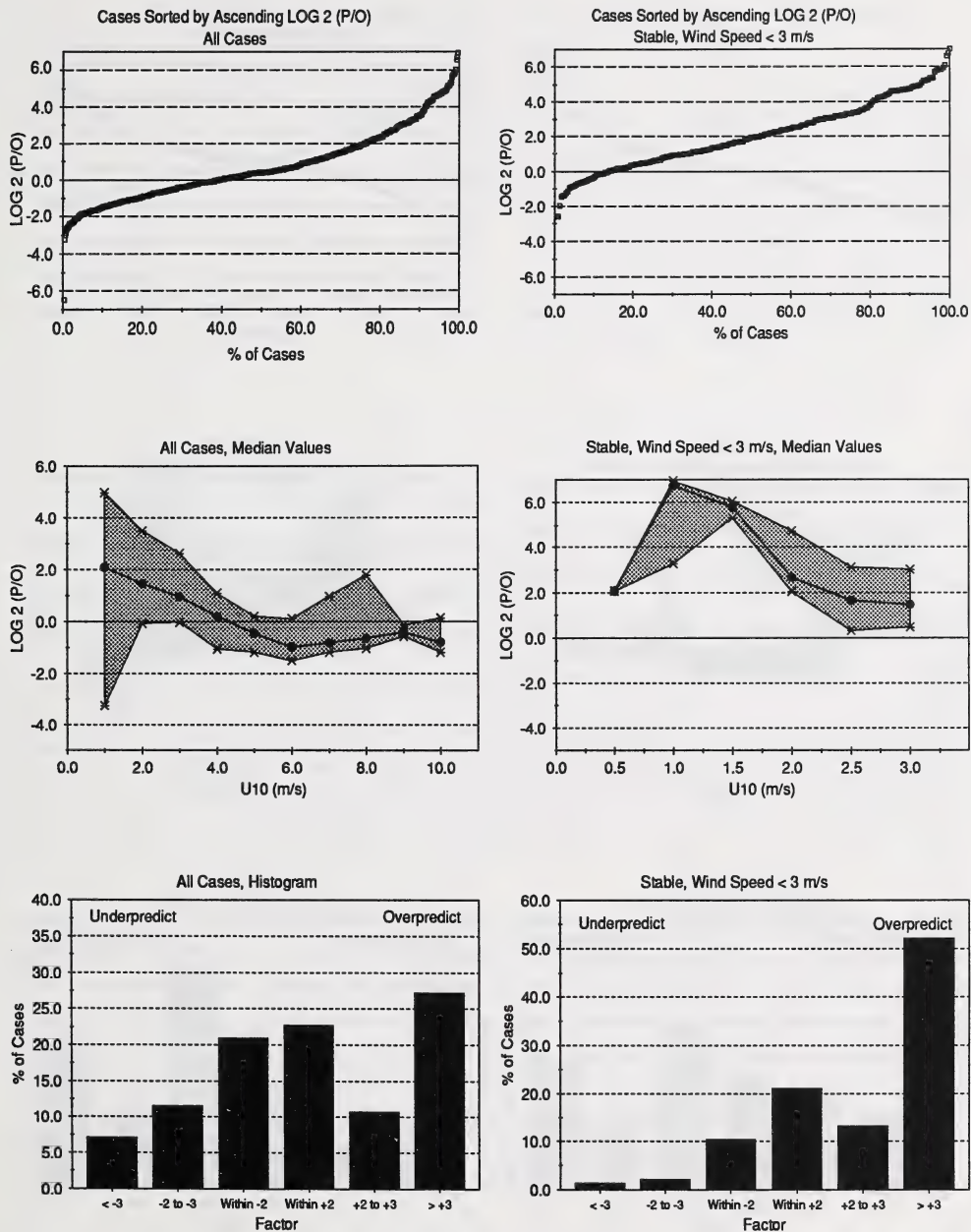


Figure C.8

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for All Cases and Stable, < 3 m/s for Option # 5 (30 second sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

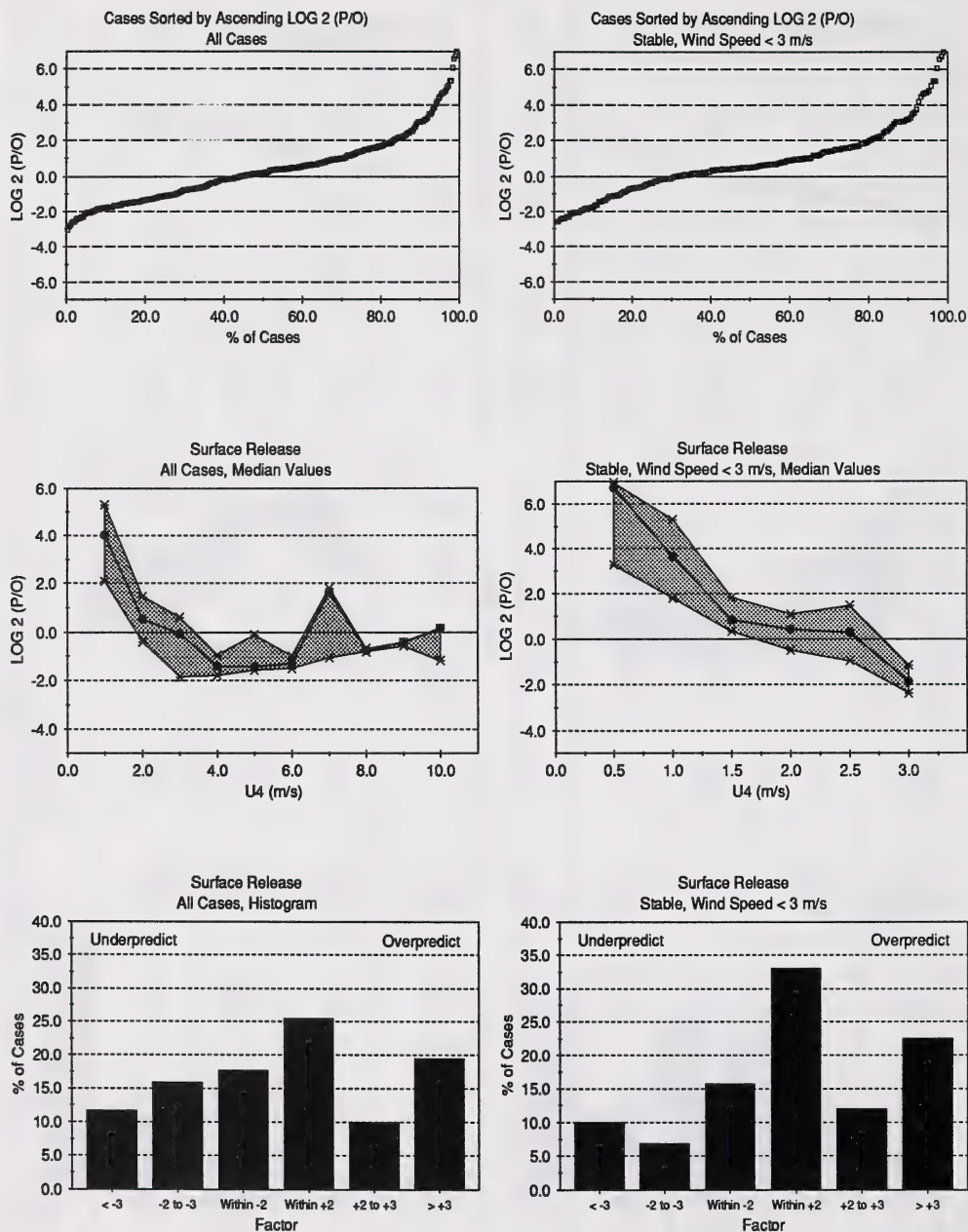


Figure C.9

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for Ground Releases and Stable, < 3 m/s for Option # 5 (30 second sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

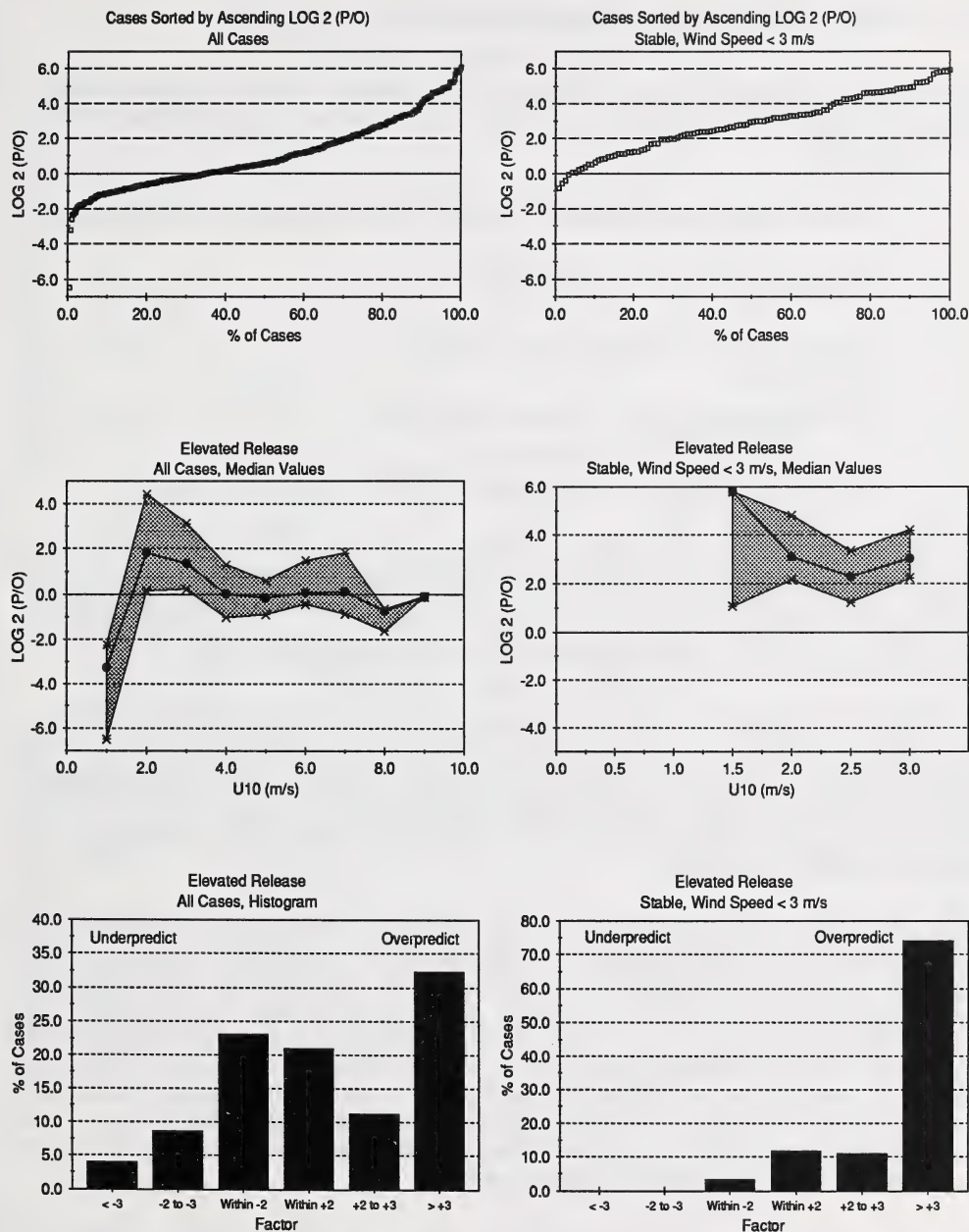


Figure C.10

Paired Simple Gaussian Model Cumulative %, Medians, and Histogram Plots for Elevated Releases and Stable, < 3 m/s for Option # 5 (30 second sigmas). The Shaded Envelope Indicates the 25 and 75 Percentile Limits.

C1.6 Model Performance - Unpaired Data

Unpaired data performance was undertaken for Option 5 model predictions only. Cumulative frequency distributions of normalized concentrations were subdivided into the following groups:

- Elevated and ground releases, 700 and 1 400 m receptor distance (all cases),
- Ground release, 700 m receptor distance,
- Ground release, 1 400 m receptor distance,
- Elevated release, 700 m receptor distance, and
- Elevated release, 1 400 m receptor distance.

The normalized concentration (χ/Q) were defined as the observed plume centreline concentration defined by the Moment Method (ppt) divided by the SF_6 source release rate (g/min). The normalization allows comparison of all traverse data even though the release rates were varied between the tests. The largest χ/Q ratios represent the lowest dilution factors and are indicative of potential "worst case" meteorological scenarios.

The fractional bias (FB) was only computed for the "all cases" data set and was based on the 25 highest normalized concentration pairs. The computed value for Option 5 is 0.101. Values of the fractional bias that are equal to -0.67 (+0.67) are equivalent to overpredictions (underpredictions) by a factor of two. Models associated with computed FB values that are between -0.67 and +0.67 are deemed to have passed an initial test for consideration as a regulatory model (Cox 1988).

Figure C.11 shows the cumulative frequency distributions for surface releases (700 and 1 400 m) for Option 5 based predictions. For the 700 m concentrations, the cumulative frequency distributions for the observed and predicted values are similar for normalized concentration values up to 4 000 ppt/(g/min). These values include 73% of the data. For normalized concentrations between 4 000 and 12 000 ppt/(g/min), the model under predicts. For normalized concentrations greater than 12 000 ppt/(g/min), the model over predicts by a factor of up to 2.5. For the 1 400 m concentrations, the cumulative frequency distributions are similar for normalized concentration values of up to 3 000 ppt/(g/min). These values include 80% of the data. For normalized concentrations greater than this value, the simple Gaussian model overpredicts by a factor of up to 2.5.

Figure C.12 shows the cumulative frequency distributions for elevated releases (700 and 1 400 m) for Option 5 predictions. For the 700 m concentrations, the simple Gaussian model overpredicts for normalized concentrations less than 150 ppt/(g/min). These values include 36% of the data. For normalized concentrations between 150 and 350 ppt/(g/min), the predicted and observed values are in agreement. For normalized concentrations greater than 350 ppt/(g/min), the simple Gaussian model tends to underpredict by a factor of up to 1.7. For the 1400 m concentrations, the model predictions and observations appear to be in agreement for normalized concentrations less than 300 ppt/(g/min). For normalized concentrations greater than this value, the model tends to underpredict by a factor of up to 2.8.

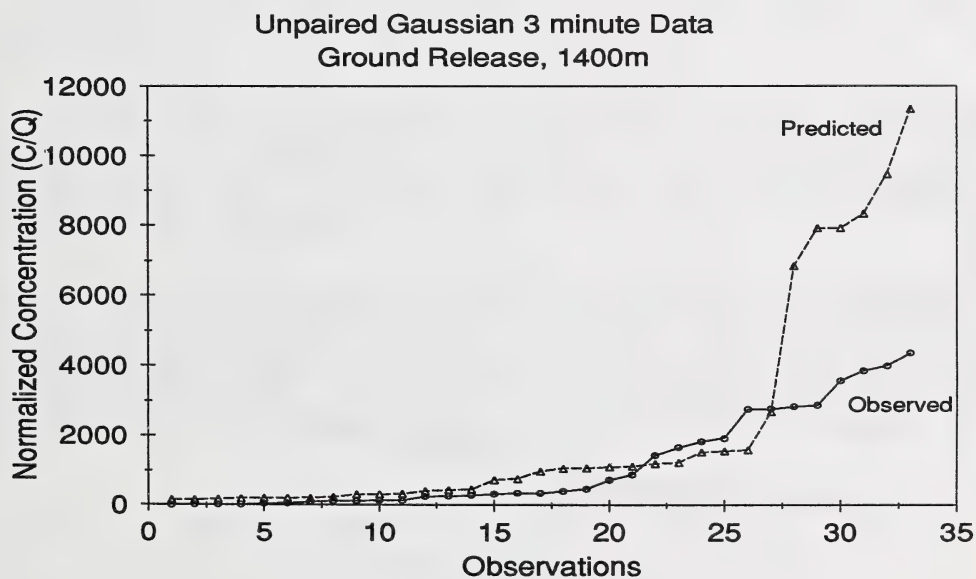
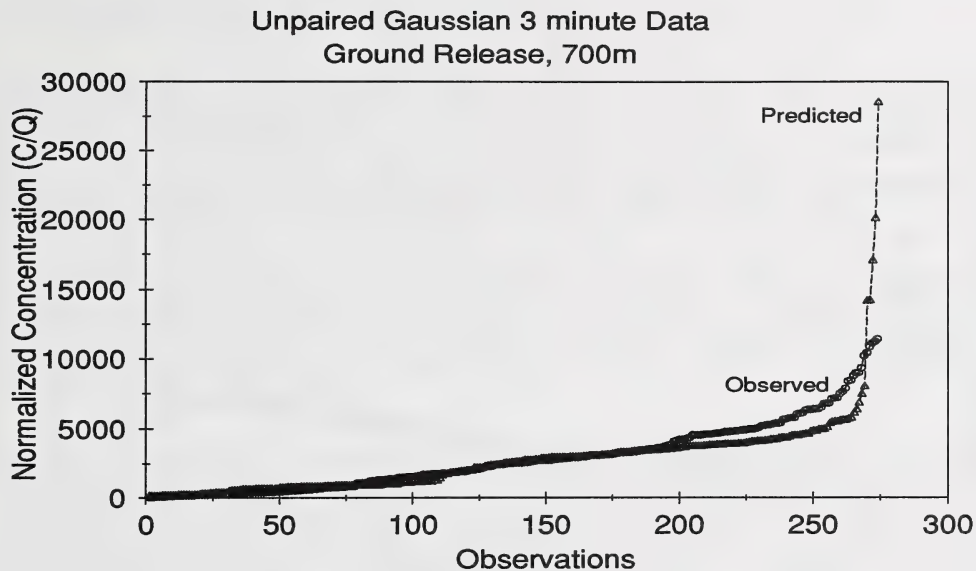


Figure C.11

Unpaired Comparison of Simple Model Predictions and Observed Centreline Concentrations (Moment Method) For All Cases During Ground Releases, Ranked Using Concentration Normalized by Release Rate.

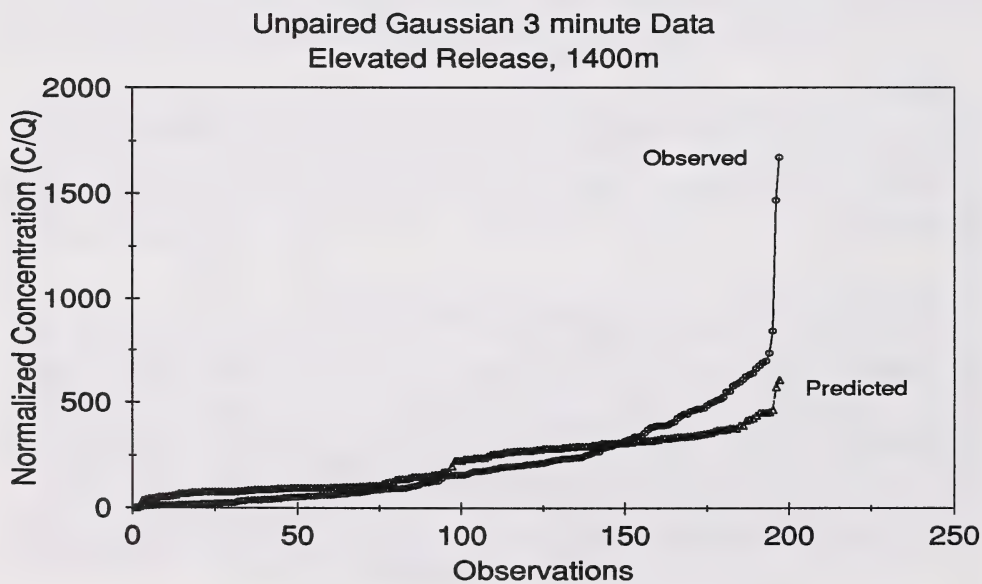
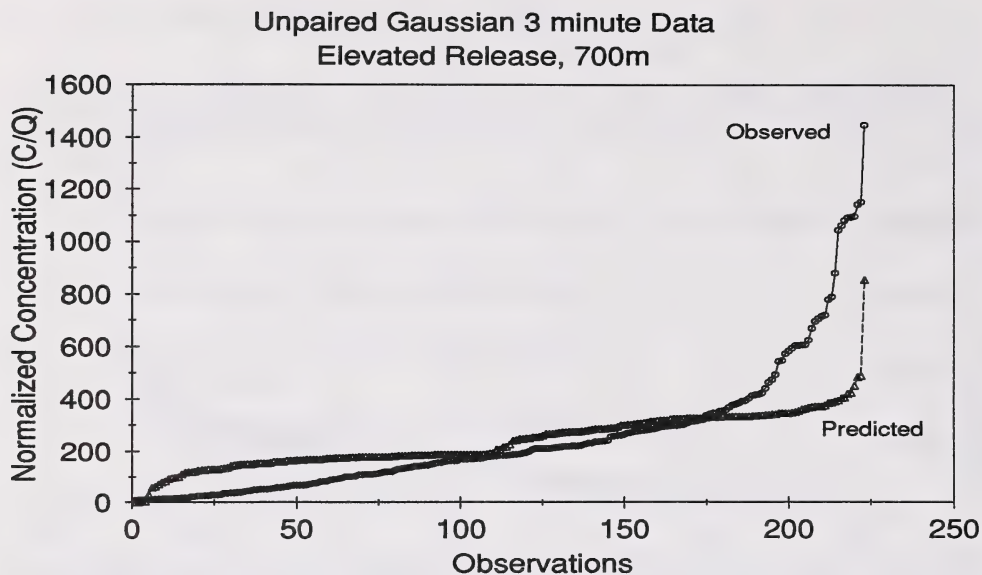


Figure C.12

Unpaired Comparison of Simple Model Predictions and Observed Centreline Concentrations (Moment Method) For All Cases During Elevated Releases, Ranked Using Concentration Normalized by Release Rate.

C1.7 Model Performance Comments

For the paired data analysis, the lowest overall simple Gaussian model performance was associated with the option which included wind direction shear. The wind shear enhancement produced larger σ_{yi} values which resulted in a consistent underprediction. For all the other options, mean and median predictions are comparable to the corresponding observations, and about 40 to 50% of the predictions are within a factor of two.

A subset of the data set based on low wind speed ($U < 3$ m/s), stable conditions were evaluated. For **ground** releases, the model tends to **under predict** by a factor of about 2.5 for options 1, 2, 3 and 5. In contrast, for **elevated** releases, the model tends to **over predict** by a factor of about 3 for all options except Option 4. For Option 4, there is better agreement between predicted and observed.

The unpaired data analysis focussed on Option 5 only. For **ground** releases, the model tended to **over predict** by a factor of up to 2.5 for the largest normalized concentrations. For the **elevated** releases, the model tends to **under predict** by a similar factor for the largest normalized concentrations. The direction of prediction tendencies are opposite to what was found for the paired analysis. Considering the difficulties in trying to pair data in time and space there is a higher degree of confidence in the unpaired data analysis. It must also be noted that for this unpaired analysis 3-minute sigma values were used. If a smaller averaging time were used to try to approximate instantaneous sigmas then the concentrations would have been higher.

These findings indicate the potential problems which may arise when using an entire data set to compare model predictions with observations. In particular, competing effects may indicate a certain level of performance that may not necessarily be indicated by a data subset. For this reason it is important to use subsets based on source type and meteorology to fully evaluate a model's performance.

Rather than pursue any further simple Gaussian model evaluation on subsets of data an effort was made to focus on the GASCON2 model. It was a lot easier to evaluate the simple model to understand whether paired or unpaired data should be used, whether the data should be split into ground or elevated or split into low and high wind speeds. Valuable information was also gained in looking at the differences when using 30-second versus 3-minute sigmas. This information was used in setting up the procedure for the GASCON2 evaluation.

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Volume 4 SYMBOL GLOSSARY

Symbol	Description	Section
A	constant, dependent upon surface roughness, used to estimate σ_x in Equation 4.113	B1.4
A_C	area of the jet at "C" plane (m^2)	B1.2.4
A_E	cross sectional area of rupture (m^2)	B1.1.2
AE	fan cross sectional area (m^2)	3.2.1
A_{EFF}	effective surface area between "Q" and "S" planes (m^2)	3.2.1
A_Q	area of the jet at "Q" plane (m^2)	B1.2.2
A_S	area of the jet at "S" plane (m^2)	B1.2.3
a	mass fraction CH_4 in sour gas	B1.2.4
a	constant used in Alberta Environment estimation of σ_y	C1.2
a_T	molar ratio of reactants to products	B1.2.4
B	constant, dependent upon surface roughness, used to estimate σ_x in Equation B1.113	B1.4
b	mass fraction H_2S in sour gas	B1.2.4
b	constant used in Alberta Environment estimation of σ_z	C1.2
b_I	strength of the inversion (m/s^2)	B1.5.1
C	concentration (ppt)	4.4.1
C_a	actual concentration (ppt)	4.2.4
C_{D1}	drag coefficient	B1.2.3
C_{D2}	drag coefficient to account for the obstruction the plume presents to the ambient flow	B1.3.1
$(C_E)_C$	concentration of combusted gas in the gas-air mixture at "C" plane (kg/m^3)	B1.2.4
C_F	skin friction coefficient of plume impinging on ground	B1.3.1
C_L	lean flammability limit of combined CH_4 - H_2S stream, fraction by volume	B1.2.4
$C_{L(CH_4)}$	CH_4 concentration at the lean flammability limit, fraction by volume (0.05)	B1.2.4
$C_{L(H_2S)}$	H_2S concentration at the lean flammability limit, fraction by volume (0.042)	B1.2.4
C_m	measured concentration (ppt)	4.2.4
C_O	speed of sound in pipeline gas before rupture (m/s)	B1.1.2
C_P	specific heat at constant pressure ($J/(kg\ K)$)	B1.2.1
C_{PA}	specific heat of air at constant pressure ($J/(kg\ K)$)	3.2.1

C_{PC}	specific heat at constant pressure of combusted gas-air mixture (J/(kg K))	B1.2.4
C_{PCO_2}	specific heat at constant pressure of CO ₂ (J/(kg K))	B1.2.4
C_{PE}	specific heat at constant pressure of the gas at "E" plane (J/(kg K))	B1.2.1
$(C_{PE})_C$	specific heat at constant pressure of combusted gas at "C" plane (J/(kg K))	B1.2.4
C_{PH_2O}	specific heat at constant pressure of H ₂ O (J/(kg K))	B1.2.4
C_{PI}	specific heat at constant pressure of gas stream "I" (J/(kg K))	Table B1.1
C_{PN_2}	specific heat at constant pressure of N ₂ (J/(kg K))	B1.2.4
C_{PO_2}	specific heat at constant pressure of O ₂ (J/(kg K))	B1.2.4
C_{PQ}	specific heat at constant pressure of the gas at "Q" plane (J/(kg K))	B1.2.2
C_{PS}	specific heat at constant pressure of the gas-air mixture at "S" plane (J/(kg K))	B1.2.3
C_{PSO_2}	specific heat at constant pressure of SO ₂ (J/(kg K))	B1.2.4
C_Q	sonic velocity at the "Q" plane	B1.2.2
$(C_{SO_2})_C$	concentration of SO ₂ in the combusted gas at "C" plane (kg/m ³)	B1.2.4
C_V	specific heat at constant volume (J/(kg K))	B1.1.2
C_{VE}	specific heat at constant volume of the gas at "E" plane (J/(kg K))	B1.2.1
c	concentration of scalar species (e.g., H ₂ S) in the plume (kg/m ³)	B1.3.1
c	exponent used in Alberta Environment estimation of σ_z	C1.2
$\dot{c}$	volumetric source/sink of scalar species in the plume due to chemical production/depletion (kg/s)	B1.3.1
c_T	molar concentration of fuel in the stoichiometric mixture	B1.2.4
d	pipeline line diameter (m)	B1.1.2
dT_A/dZ	vertical temperature gradient in the atmosphere	B1.3.3
F	pipeline friction factor	B1.1.2
F_B	bouyancy flux (m ⁴ /s ³)	3.1
F_M	momentum flux (m ⁴ /s ²)	B1.3.2
F_{RS}	Froude number with combustion	B1.2.4
f	fraction of the plume remaining in the mixed layer	3.1
f_A	factor to account for plume cross-sectional area reduction due to ground impingement	B1.3.1

f_{CY}	dimensionless correction factor to force the Weil and Brower σ_Y values to equal the Briggs (1974) σ_Y values at large distances	B1.5.2
f_{CZ}	dimensionless correction factor to force the Weil and Brower σ_Z values to equal the Briggs (1974) σ_Z values at large distances	B1.5.2
f_E	factor to account for plume circumferential area reduction due to ground impingement	B1.3.1
f_{EDGE}	entrainment value to define f_{MIN}	B1.5.1
f_{MIN}	minimum value of f	B1.5.1
f_R	fraction of heat produced by combustion which is lost by radiation	B1.2.4
$f_Y(x)$	dimensionless function which relates cross wind velocity fluctuations to cross wind plume spread	B1.5.2
$f_Z(x)$	dimensionless function which relates vertical wind velocity fluctuations to vertical plume spread	B1.5.2
g	acceleration of gravity	C1.1
g	function to account for vertical plume spreads	3.1
g_1	function to account for plume reflections from ground	3.1
g_2	function to account for plume reflections from inversion at mixed layer height Z_i	3.1
g_3	function to account for uniform mixing of plume within mixed layer Z_i	3.1
H	plume height (m)	C1.1
H_o	surface heat flux (W/m^2)	3.1
h_s	source height (m)	C1.1
Δh	Briggs' final plume rise (m)	B1.3.3
Δh_B	final bouyancy rise (m)	B1.3.3
$(\Delta h_B)_N$	final bouyancy rise in neutral conditions (m)	B1.3.3
$(\Delta h_B)_S$	final bouyancy rise in stable conditions (m)	B1.3.3
$(\Delta h_B)_U$	final bouyancy rise in unstable conditions (m)	B1.3.3
Δh_M	final momentum rise (m)	B1.3.3
Δh_{SC}	stable plume rise relationship applicable to near calm conditions (m)	B1.3.3
Δh_1	"sum of cubes" final rise for non-calm conditions (m)	B1.3.3
Δh_2	"sum of cubes" final rise for near calm conditions (m)	B1.3.3

I_1	first term in analytical expression for the effective mass release rate	Table B1.6
I_2	second term in analytical expression for the effective mass release rate	Table B1.6
I_3	third term in analytical expression for the effective mass release rate	Table B1.6
k	von Karman constant	B1.3.3
k_C	ratio of specific heats for the combusted gas-air mixture (C_P/C_V) at "C" plane	B1.2.4
k_E	ratio of specific heats for the pipeline gas (C_P/C_V)	B1.1.2
k_Q	ratio of specific heats for the pipeline gas (C_P/C_V) at "Q" plane	B1.2.2
k_S	ratio of specific heats for the gas-air mixture (C_P/C_V) at "S" plane	B1.2.3
L	Monin-Obukhov length (m)	1.6
L_C	length between "S" and "C" planes (m)	Figure B1.2
L_Q	jet length between "E" and "Q" planes (m)	Figure B1.2
L_S	jet length between "Q" and "S" planes (m)	Figure B1.2
L_{ST}	time zone standard longitude (degrees)	Table 3.1
L_T	latitude of site (degrees)	Table 3.1
l	pipeline length (m)	B1.1.2
l_{EFF}	effective pipeline length to allow for the extra gas released during the time taken for the ESD valves to fully close	B1.1.2
M_S	Mach number	B1.2.3
MSE	mean square error	4.3.2
M_T	total mass to be released (kg)	B1.1.2
M_{WA}	molecular weight of air (28.95 kg/kmole)	B1.2.3
M_{WC}	molecular weight of combusted gas-air mixture at "C" plane (kg/kmole)	B1.2.4
M_{WCO_2}	molecular weight of CO ₂ (44 kg/kmole)	B1.2.4
M_{WE}	molecular weight of the discharging gas at "E" plane (kg/kmole)	B1.2.1
$(M_{WE})_C$	molecular weight of combusted gas at "C" plane (kg/kmole)	B1.2.4
M_{WH_2O}	molecular weight of H ₂ O (18 kg/kmole)	B1.2.4
M_{WI}	molecular weight of gas stream "I" (kg/kmole)	Table B1.1
M_{WN_2}	molecular weight of N ₂ (28 kg/kmole)	B1.2.4
M_{WO_2}	molecular weight of O ₂ (32 kg/kmole)	B1.2.4

M_{WQ}	molecular weight of the gas at "Q" plane (kg/kmole)	B1.2.2
M_{WS}	molecular weight of the gas-air mixture at "S" plane (kg/kmole)	B1.2.3
M_{WSF_6}	molecular weight of SF ₆ (146.06 kg/kmole)	3.1
M_{WSO_2}	molecular weight of SO ₂ (64 kg/kmole)	B1.2.4
$\dot{m}_A$	mass flow of air entrained between "Q" plane and "S" plane (kg/s)	B1.2.3
$(\dot{m}_A)_C$	mass flow of air at "C" plane (kg/s)	B1.2.4
$\dot{m}_{AC}$	mass flow of air entrained between "S" plane and "C" plane (kg/s)	B1.2.4
$\dot{m}_C$	mass flow of combusted gas-air mixture at "C" plane (kg/s)	B1.2.4
$\dot{m}_{air}$	steady mass flow rate of air (kg/s)	3.2.1
$(\dot{m}_C)_{CO_2}$	mass flow of CO ₂ at "C" plane (kg/s)	B1.2.4
$(\dot{m}_C)_{H_2O}$	mass flow of H ₂ O at "C" plane (kg/s)	B1.2.4
$(\dot{m}_C)_{N_2}$	mass flow of N ₂ at "C" plane (kg/s)	B1.2.4
$(\dot{m}_C)_{O_2}$	mass flow of O ₂ at "C" plane (kg/s)	B1.2.4
$(\dot{m}_C)_{SO_2}$	mass flow of SO ₂ at "C" plane (kg/s)	B1.2.4
$\dot{m}_E$	mass flow rate of gas at "E" plane (kg/s)	B1.1.1
$(\dot{m}_E)_C$	mass flow of combusted gas at "C" plane (kg/s)	B1.2.4
$\dot{m}_E(t)$	mass release rate at time t (kg/s)	B1.1.3
$\dot{m}_E(\tau)$	mass release rate at time τ (kg/s)	B1.4
$\dot{m}_{EFF}(x_1, t)$	effective mass flux at distance x_1 which accounts for along wind diffusion (kg/s)	B1.4
$\dot{m}_{E,S}$	steady state mass release rate portion	B1.1.3
$\dot{m}_{E,T}(t)$	transient mass release rate portion at time t	B1.1.3
$\dot{m}_0$	initial gas release rate at time $t=0$ s (kg/s)	B1.1.2
$\dot{m}_p$	mass flow rate of the given plume component (H ₂ S or SO ₂) in the release (kg/s)	B1.5.2

$\dot{m}_Q$	mass flow of gas at the "Q" plane	B1.2.3
$\dot{m}_S$	mass flow of gas-air mixture through the "S" plane (kg/s)	B1.2.3
$\dot{m}_{SF_6}$	mass flow rate of sulphur hexafluoride (kg/s)	3.1
N	number of observations	4.3.2
n	constant, dependent upon surface roughness, used to estimate σ_x	B1.4
O	observed value	4.3.2
$\overline{O}$	mean observed value	4.3.2
P	bouyancy parameter used to determine fraction of the plume remaining in the mixed layer for unstable conditions	B1.5.1
P	predicted value	4.3.2
$\overline{P}$	mean predicted value	4.3.2
P_A	surface pressure (kPa)	B1.2.1
P_{amb}	ambient pressure (kPa)	3.1
P_c	calibration pressure (kPa)	3.2.1
P_E	pressure of the gas at "E" plane (kPa)	B1.2.1
P_O	gas pressure in pipeline before rupture (P_A)	B1.1.2
P_Q	pressure of the gas at "Q" plane (kPa)	B1.2.2
P_S	pressure of the gas-air mixture at "S" plane (kPa)	B1.2.3
P_{st}	standard pressure (kPa)	3.2.1
p	cross-wind sigma power law exponent	4.4.4
ppt	parts per trillion	C1.1
Q	mass flow rate of SF_6 (g/min)	4.4.1
Q	SF_6 release rate (m^3/s)	C1.1
Q_H	heat produced by the combustion reaction (J/m^3)	B1.2.4
Q_{HI}	heat of combustion of gas stream "I" (J/m^3)	Table B1.1
q	averaging time correction exponent, dependent upon atmospheric stability	B1.5.4
$\dot{q}$	volumetric source/sink of energy in the plume. At present $\dot{q}$ is assumed to be zero (W/m^3)	B1.3.1
R_C	particular gas constant of the combusted gas-air mixture at "C" plane ($J/(kg\ K)$)	B1.2.4
R_E	particular gas constant at "E" plane ($J/(kg\ K)$)	B1.1.1
$(R_E)_C$	particular gas constant of the combusted gas at "C" plane ($J/(kg\ K)$)	B1.2.4
R_I	particular gas constant for gas stream "I" ($J/(kg\ K)$)	Table B1.1

R_Q	particular gas constant at "Q" plane (J/(kg K))	B1.2.2
R_S	particular gas constant of the gas-air mixture at "S" plane (J/(kg K))	B1.2.3
R_U	universal gas constant (8314 J/(kmole K))	Table B1.1
r	plume radius (m)	B1.3.1
r	correlation coefficient	Table C.2
r_F	plume radius at the downwind distance X_F (m)	B1.5.2
r_{ST}	radius of the stack (m)	Table 5.28
S	stability parameter used for estimating plume rise in stable conditions (s^{-2})	C1.1
S_d^2	variance of the difference	4.3.2
S_{REF}	combination of some of the parameters used to estimate the Pasquill-Smith horizontal plume spread $= \sigma_{YREF} \left(\frac{1}{x_{REF}} \right)^{P_Y}$ (see Table 5.29)	B1.2.4
S_O	square of the Brunt-Vaisala frequency (s^{-2})	B1.3.3
s	plume centerline coordinate (m)	B1.3.1
T	plume temperature (K)	B1.3.1
T	ambient temperature (K)	C1.1
T_{amb}	ambient temperature (K)	3.1
T_C	temperature of the combusted gas-air mixture at "C" plane (K)	B1.2.4
T_C	calibration temperature (K)	3.2.1
T_E	temperature of the gas at "E" plane (K)	B1.2.1
T_O	temperature of gas in pipeline before rupture (K)	B1.1.2
T_Q	temperature of the gas at "Q" plane (K)	B1.2.2
T_S	temperature of the gas-air mixture at "S" plane (K)	B1.2.3
T_{st}	standard temperature (K)	3.1
t	time	
t	duration of concentration Ca	4.2.4
t_1	averaging time (s)	4.4.2
t_2	averaging time (s)	4.4.2
t_s	time at which the steady state mass release rate dominates in a continuous pipeline release (s)	B1.1.3
U	ambient windspeed (varies with z) (m/s)	C1.1
$\overline{U}$	mean transport wind speed of the plume (m/s)	3.1
$U(z)$	wind speed at height z (m/s)	B1.4

U^*	surface friction velocity (m/s)	1.6
U_C	ambient wind speed at height of "C" plane (m/s)	B1.2.4
U_{Fan}	fan velocity (m/s)	3.2.1
U_P	wind speed at plume height (m/s)	3.1
U_Q	ambient wind speed at height of "Q" plane (m/s)	B1.2.3
U_{REF}	wind speed at anemometer height (m/s)	B1.3.4
U_S	ambient wind speed at height of "S" plane (m/s)	B1.2.4
V	plume velocity (m/s)	B1.3.1
$\dot{V}$	volume flow rate of sour gas (m ³ /d)	B1.1.1
V_C	velocity of the combusted gas-air mixture at "C" plane (m/s)	B1.2.4
V_{CH_4}	volume fraction CH ₄ in the escaping gas	B1.2.4
V_{CO_2}	volume fraction CO ₂ in the escaping gas	B1.2.4
V_α	entrainment velocity, for parameterizing the amount of ambient air which is entrained into the plume (m/s)	B1.3.1
V_E	velocity of the gas at "E" plane (m/s)	B1.2.1
V_{EFF}	effective tangential velocity difference (m/s)	B1.2.3
V_{H_2S}	volume fraction H ₂ S in the escaping gas	B1.2.4
V_Q	velocity of the gas at "Q" plane (m/s)	B1.2.2
V_R	relative velocity between the plume and the atmosphere (m/s)	B1.3.1
V_S	velocity of the gas-air mixture at "S" plane (m/s)	B1.2.3
V_S	exit velocity of the jet (m/s)	C1.1
$\dot{V}_{SF_6}$	volumetric flow of a given plume component (SF ₆) in the release at ambient conditions (m ³ /s)	3.1
V_{SZ}	vertical component of V_S (m/s)	Table B1.4
V_X	horizontal velocity component of plume (m/s)	B1.3.1
V_Z	vertical velocity component of plume (m/s)	B1.3.1
$W''T'$	10 m heat flux product (K · m/s)	3.2.1
W^*	convective velocity scale (m/s)	B1.3.3
WDE	wind shear direction enhancement	C1.2
X_O	virtual distance to account for a non-zero ground release in the estimation of vertical exponential profile (m)	B1.5.3
X_{SY}	distance from a virtual y-source (m)	B1.5.2
X_{SZ}	distance from a virtual z-source (m)	B1.5.2
X_{VY}	virtual distance to account for the spread of the plume in the cross wind direction (m)	Table B1.7

X_{VZ}	virtual distance to account for the spread of the plume in the vertical direction (m)	Table B1.7
X^*_O	non-dimensional virtual distance to account for a non-zero ground release in the estimation of vertical exponential profile (m)	B1.5.3
X^*_{SY}	non-dimensional distance from a virtual y-source for surface plumes	B1.5.3
X^*_{SZ}	non-dimensional distance from a virtual z-source for surface plumes	B1.5.3
X^*_{VY}	non-dimensional virtual distance to account for the spread of the plume in the cross wind direction for surface plumes	B1.5.3
x	horizontal coordinate or downwind distance (m)	C1.2
x_F	downwind distance from rupture point when integral plume rise model is terminated (m)	B1.3.2
x_S	virtual distance (m)	B1.3.2
x_V	distance calculated by forcing Equation B1.92 for Z_p to recover Z_F at $x=x_F$ (m)	B1.3.2
y	cross wind distance (m)	3.1
$\bar{Z}$	mean height to which plume has dispersed (m)	3.1
Z_C	elevation of "C" plane above the ground (m)	Figure B1.2
$\tilde{Z}_C$	pipeline gas compressibility prior to rupture	B1.1.2
Z_E	elevation of "E" plane above the ground (m)	Figure B1.2
$\tilde{Z}_E$	gas compressibility at the exit	B1.1.2
Z_F	plume elevation when the integral plume rise model is terminated (m)	B1.3.2
Z_i	mixing height (m)	3.1
Z_M	height to estimate stability parameter for plume rise evaluation (m)	B1.3.3
Z_O	surface roughness length (m)	B1.5.3
Z_P	plume elevation (m)	3.1
Z_{PF}	final plume elevation above ground level or in the case of partial plume penetration, the height of the remaining portion of the plume in the mixed layer (m)	B1.3.3
$Z_{PF,BRIGGS}$	Briggs' final plume elevation (m)	B1.3.3
$Z_{PF,PEN}$	final elevation of the plume if plume penetration is predicted (m)	B1.5.1
Z_Q	elevation of "Q" plane above the ground (m)	Figure B1.2
Z_R	function used to estimate σ_x (m)	B1.4
Z_{REF}	anemometer height (m)	B1.3.3
Z_S	elevation of "S" plane above the ground (m)	Figure B1.2

Z_{sc}	plume elevation for near calm conditions (m)	B1.3.3
Z_v	function used to estimate σ_x (m)	B1.4
z	height above ground level (m)	3.1
$\frac{\partial T}{\partial Z}$	vertical temperature gradient (K/m)	C1.1

Greek Symbol	Description	Section
α	entrainment constant in Equation B1.38	B1.2.3
α_2	constant, dependent upon surface roughness, used to estimate σ_x in Equation B1.113	B1.4
β	entrainment velocity parameter in Equation B1.90	B1.3.1
Γ	inertial delay factor	B1.1.2
Γ	adiabatic temperature gradient (0.0098 K/m)	C1.1
δ	height of plume centerline above the ground (m)	B1.3.1
ε	time constant in Equation B1.4 (s)	B1.1.2
η	mass conservation factor	B1.1.2
θ	potential temperature of plume (K)	B1.3.1
θ_A	potential temperature of the atmosphere (varies with z depending upon stability) (K)	B1.3.1
$\Delta\theta_i$	change in potential temperature across the depth of the inversion	B1.5.1
$\partial\theta/\partial Z$	potential temperature gradient (K/m)	B1.3.3
λ	angle of jet with horizontal (degrees)	B1.2.3
ρ	density of plume (kg/m^3)	B1.3.1
ρ_A	ambient air density (varies with z) (kg/m^3)	3.1
ρ_C	density of the combusted gas-air mixture at "C" plane (kg/m^3)	B1.2.4
ρ_C	calibration air density (kg/m^3)	3.2.1
ρ_E	density of the gas at "E" plane (kg/m^3)	B1.2.1
ρ_{EO}	density of sour gas at standard conditions of 15 °C and 101.3 kPa	B1.2.4
ρ_Q	density of the gas at "Q" plane (kg/m^3)	B1.2.2
ρ_S	density of the gas-air mixture at "S" plane (kg/m^3)	B1.2.3
ρ_s	density of gas effluent at source (kg/m^3)	3.1
$\bar{\rho}$	density of sour gas at standard conditions (kg/m^3)	B1.1.1
σ	represents the growth rate of the plume between the "S" and "C" planes due to atmospheric and combustion generated turbulence	B1.2.4
σ_C	standard deviation of the plume spread at the "C" plane	B1.2.4
σ_{PS}	Pasquill-Smith horizontal plume spread (m)	B1.2.4
σ_S	represents the "initial dilution" at the "S" plane	B1.2.4
σ_V	standard deviation of the cross wind speed fluctuations (radian)	B1.5.2
σ_V	standard deviation of the cross-wind component (m)	1.6

σ_w	standard deviation of the vertical wind speed fluctuations (radian)	B1.5.2
σ_w	standard deviation of vertical-wind component (m)	1.6
σ_x	standard deviation of the transient plume in the along wind direction (m)	B1.4
σ_θ	standard deviation of wind direction (°)	Table 3.1
σ_Y	standard deviation of the plume in the cross wind direction (m)	3.1
σ_{Y1}	horizontal plume spread for averaging time t_1 (m)	4.4.4
σ_{Y2}	horizontal plume spread for averaging time t_2 (m)	4.4.4
σ_ϕ	standard deviation of the vertical wind angle (°)	Table 3.1
σ_z	standard deviation of the plume in the vertical direction (m)	1.6
τ	analyser response time	4.3.2
τ	lagged time after release used to calculate the transient mass release rate (s)	B1.4
ϕ	plume angle with respect to the ground. defined in Equation B1.88	B1.3.1
χ	concentration in gaussian formulation (often used interchangeably with C) (ppt)	C1.1
$\chi(x,0,0)$	concentration of a given plume component (H_2S or SO_2) at position $(x,0,0)$ (kg/m^3)	B1.5.2
$\chi(x,y,z)$	concentration of a given plume component (H_2S or SO_2) at position (x,y,z) (kg/m^3)	B1.5.2
$\chi(x,y,z)$	concentration of a given plume component (SF_6) at position (x,y,z) (ppt)	3.1
χ_3	three minute average concentration (assumed to be instantaneous for transient releases) (kg/m^3)	B1.5.4
χ_{60}	60 minute average concentration (kg/m^3)	B1.5.4

Symbol**Chemical Symbols**

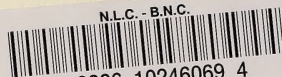
CH ₄	methane
CO ₂	carbon dioxide
H ₂ O	water
H ₂ S	hydrogen sulphide
N ₂	nitrogen
O ₂	oxygen
SO ₂	sulphur dioxide
SF ₆	Sulphur hexafluoride

Subscripts

<i>U</i>	natural wind coordinate, along-wind component
<i>V</i>	natural wind coordinate, cross-wind component
<i>W</i>	natural wind coordinate, vertical-wind component
<i>4</i>	4m level
<i>10</i>	10m level
<i>16</i>	16m level
<i>25</i>	25m level



N.L.C. - B.N.C.



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